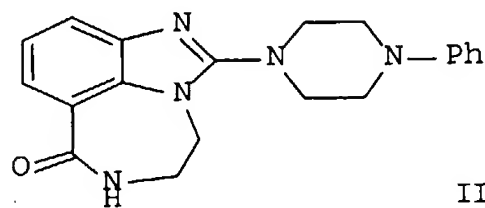
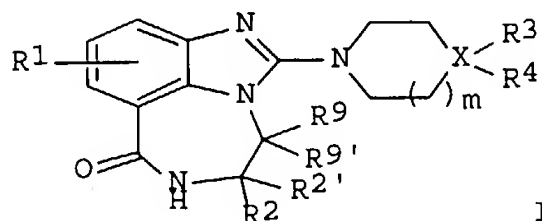


L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:408675 CAPLUS Full-text  
 DN 136:401791  
 TI Benzimidazole derivatives, specifically imidazo[4,5,1-j,k][1,4]benzodiazepin-7(4H)-one derivatives, and the preparation and therapeutic use thereof as inhibitors of poly(ADP-ribose)polymerase (PARP).  
 IN Barth, Francis; Bichon, Daniel; Bolkenius, Frank; Van Dorsselaer, Viviane  
 PA Sanofi-Synthelabo, Fr.  
 SO PCT Int. Appl., 48 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA French  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002042306	A1	20020530	WO 2001-FR3667	20011121
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	FR 2816941	A1	20020524	FR 2000-15141	20001123
	FR 2816941	B1	20030131		
	FR 2816942	A1	20020524	FR 2001-6157	20010510
	FR 2816942	B1	20030509		
	AU 2002022003	A5	20020603	AU 2002-22003	20011121
	EP 1339719	A1	20030903	EP 2001-997491	20011121
	EP 1339719	B1	20040616		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004514678	T2	20040520	JP 2002-544440	20011121
	AT 269335	E	20040715	AT 2001-997491	20011121
	US 2004029866	A1	20040212	US 2003-432672	20030523
PRAI	FR 2000-15141	A	20001123		
	FR 2001-6157	A	20010510		
	WO 2001-FR3667	W	20011121		
OS	MARPAT 136:401791				
GI					



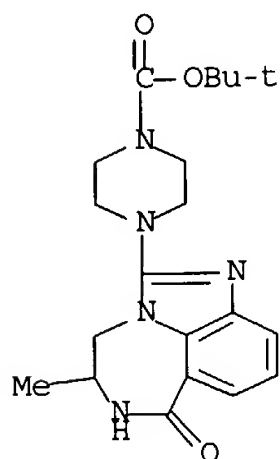
AB The invention concerns fused benzimidazole derivs. I, including their enantiomers, diastereomers, mixts., racemates, free bases, and pharmaceutically acceptable acid addition salts [wherein: R1 = H, C1-4 alkyl or alkoxy, halo, NO2; R2, R2', R9, R9' = H, C1-4 alkyl; X = N or

C; m = 1 or 2; when X = N, then R3 = H, C1-C4 alkyl, or is absent, and R4 = in particular H, C1-C6 alkyl, C3-C7 cycloalkyl, (un)substituted 4-piperidyl, (CH2)pNR5R6, (CH2)pCONR5R6, CO(CH2)pNR5R6, (un)substituted (CH2)pPh, (CH2)p-morpholinyl, (CH2)p-pyrrolidinyl, (CH2)p-tetrahydroisoquinoline, (CH2)p-heteroaryl, heteroarylcarbonyl, phenylcarbonyl, C1-C6 alkylcarbonyl, (CH2)pCOOR', or SO2Ph; when X = C, then R3 = H, NR5R6, NHCOR7, CONHR5, COR7, NHCONH2, OH, or CH2OH, and R4 = in particular H, (un)substituted (CH2)pPh, (CH2)p-heteroaryl, or (CH2)tNR7R8; p = 0-4; t = 0 or 1; R5, R6 = H, C1-4 alkyl; R7, R8 = C1-4 alkyl or alkoxy, or may together form an (un)substituted saturated ring of 5-7 members, optionally containing an addnl. N atom]. I can be used for preparing medicines for treating or preventing a wide variety of disorders wherein the PARP enzyme is involved. A table of 38 compds. I and salts is given. For instance, 4H-imidazo[4,5,1-ij]quinolin-2,6(1H,5H)-dione underwent chlorination of the 2-oxo group with POCl3 and NH4Cl, and then ring-expansion at the 6-oxo group using NaN3 and H2SO4. The resultant intermediate, 2-chloro-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, reacted with 1-phenylpiperazine in the presence of 2,6-lutidine and CsF, in triethylene glycol monomethyl ether at 140°, to give title compound II in 53% yield. The most active compds. I inhibited human recombinant PARP-1 and/or PARP-2 in vitro with IC50 values of 5-500 nM.

IT 429689-48-5P, 2-[4-[(tert-Butyloxy)carbonyl]piperazin-1-yl]-5-methyl-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (drug candidate; preparation of benzimidazole derivs. as PARP inhibitors)

RN 429689-48-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(4,5,6,7-tetrahydro-5-methyl-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT 429689-42-9P, 2-(4-Phenylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-43-0P,  
 2-[4-(4-Pyridyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-44-1P,  
 2-[4-(1-Piperidyl)piperidin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-45-2P,  
 2-[4-(5-Methyl-1H-imidazol-4-yl)piperidin-1-yl]-5,6-dihydroimidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one 429689-46-3P,  
 2-(4-Phenylpiperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-

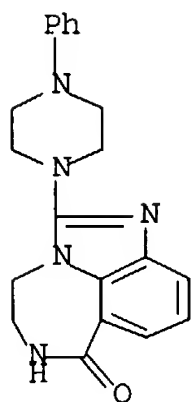
jk] [1,4]benzodiazepin-7(4H)-one 429689-47-4P,  
 2-(4-Methylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-  
 7(4H)-one 429689-49-6P, 2-[4-(2-Pyridyl)piperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-50-9P  
 , 2-(Piperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one dihydrochloride 429689-51-0P,  
 2-(4-Acetylpiperazin-1-yl)-5-methyl-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-52-1P,  
 2-[4-(4-Nitrophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-53-2P,  
 2-[4-(4-Fluorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-54-3P,  
 2-[4-(2-Chlorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-55-4P,  
 2-(4-Methylhomopiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-56-5P,  
 2-[4-[(tert-Butyloxy)carbonyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-57-6P,  
 2-(Piperazin-1-yl)-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-  
 one dihydrochloride 429689-58-7P, 2-[4-Phenyl-4-[(tert-  
 butyloxy)carbonyl]aminopiperidin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-59-8P,  
 2-[4-(2-Morpholinoethyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-60-1P,  
 2-[4-(1-Methylpiperidin-4-yl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-61-2P,  
 2-(4-Phenyl-4-aminopiperidin-1-yl)-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one dihydrochloride 429689-62-3P,  
 2-[4-[(Diethylamino)carbonyl]methyl]piperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-63-4P  
 , 2-[4-(3-Pyrrolidinopropyl)homopiperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-64-5P,  
 2-[4-[3-(Dimethylamino)propyl]piperazin-1-yl]-5-methyl-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-65-6P  
 , 2-[4-[(4-Pyridinyl)methyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-66-7P,  
 2-[4-[4-(Trifluoromethyl)phenyl]piperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-67-8P,  
 2-[4-(3-Phenylpropyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-68-9P,  
 2-[4-(2-Fluorophenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-69-0P,  
 2-[4-[(3,5-Dimethyl-1-phenylpyrazol-4-yl)methyl]piperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-70-3P  
 , 2-[4-[5-(4-Fluorophenyl)pyrazol-3-yl]piperidin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-71-4P  
 , 2-(4-Cyclohexylpiperazin-1-yl)-5,6-dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-72-5P,  
 2-[4-[3-(1,2,3,4-Tetrahydroisoquinolin-2-yl)propyl]piperazin-1-yl]-5,6-  
 dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-73-6P  
 , 2-[4-(4-Fluorophenyl)piperazin-1-yl]-10-methyl-5,6-  
 dihydroimidazo[4,5,1-  
 jk] [1,4]benzodiazepin-7(4H)-one 429689-74-7P,  
 2-(4-Cyclohexylpiperazin-1-yl)-10-methyl-5,6-dihydroimidazo[4,5,1-

jk] [1,4]benzodiazepin-7(4H)-one 429689-75-8P,  
 2-[4-(4-Fluorophenyl)piperazin-1-yl]-8-methyl-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-76-9P,  
 2-[4-(4-Fluorophenyl)piperazin-1-yl]-9-methyl-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-77-0P,  
 2-[4-(4-Fluorophenyl)piperazin-1-yl]-4-propyl-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-78-1P,  
 2-[4-[(Dimethylamino)acetyl]piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one 429689-79-2P,  
 2-[4-(4-Hydroxyphenyl)piperazin-1-yl]-5,6-dihydroimidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of benzimidazole derivs. as PARP inhibitors)

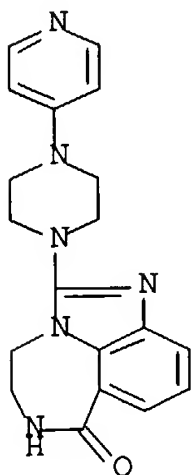
RN 429689-42-9 CAPLUS

CN Imidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



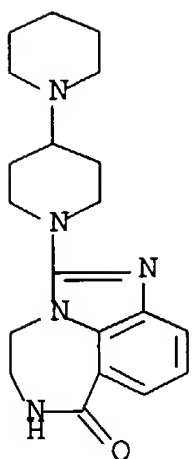
RN 429689-43-0 CAPLUS

CN Imidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



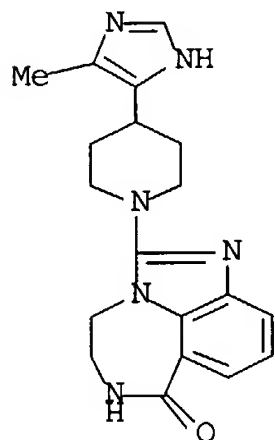
RN 429689-44-1 CAPLUS

CN Imidazo[4,5,1-jk] [1,4]benzodiazepin-7(4H)-one, 2-[1,4'-bipiperidin]-1'-yl-5,6-dihydro- (9CI) (CA INDEX NAME)



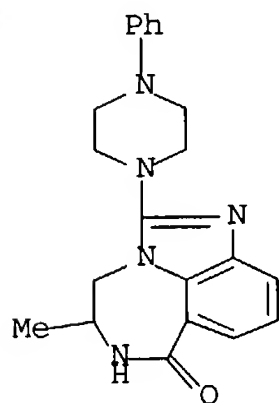
RN 429689-45-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(5-methyl-1H-imidazol-4-yl)-1-piperidinyl]- (9CI) (CA INDEX NAME)



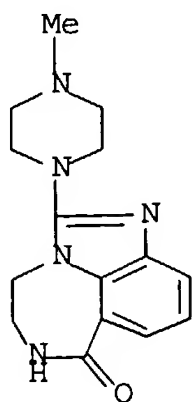
RN 429689-46-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-(4-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



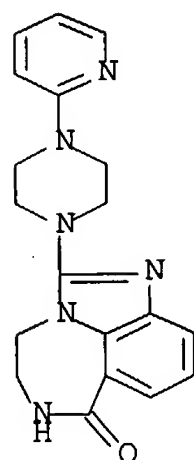
RN 429689-47-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



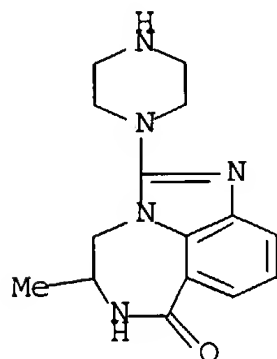
RN 429689-49-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(2-pyridinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 429689-50-9 CAPLUS

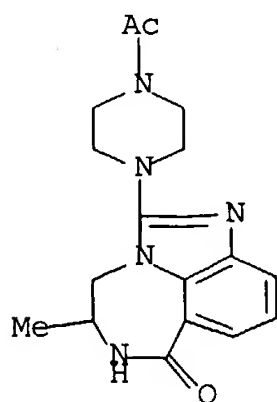
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-5-methyl-2-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

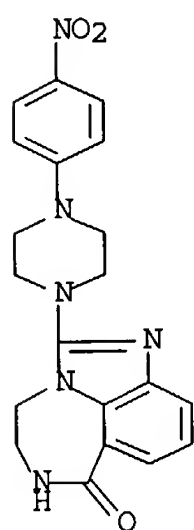
RN 429689-51-0 CAPLUS

CN Piperazine, 1-acetyl-4-(4,5,6,7-tetrahydro-5-methyl-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)



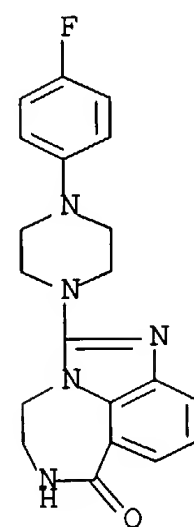
RN 429689-52-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-nitrophenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



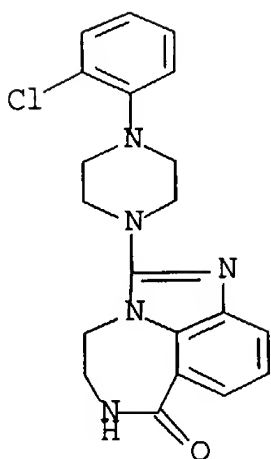
RN 429689-53-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



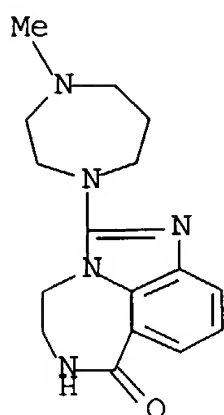
RN 429689-54-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-chlorophenyl)-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



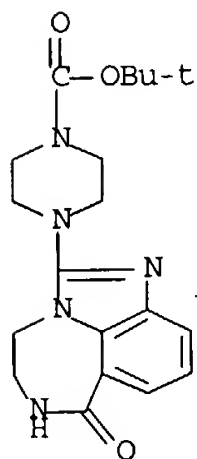
RN 429689-55-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(hexahydro-4-methyl-1H-1,4-diazepin-1-yl)-5,6-dihydro- (9CI) (CA INDEX NAME)



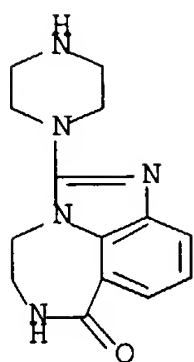
RN 429689-56-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 429689-57-6 CAPLUS

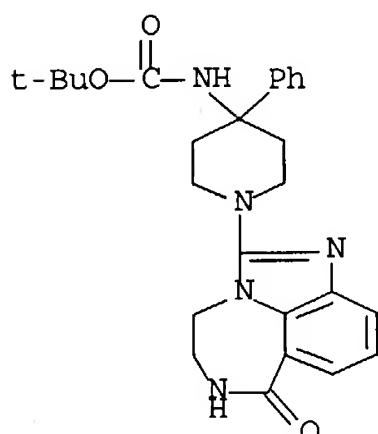
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

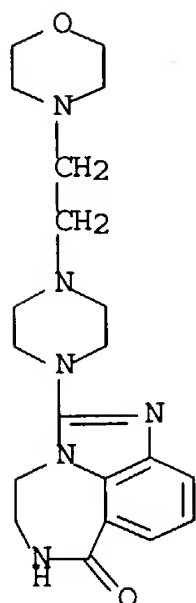
RN 429689-58-7 CAPLUS

CN Carbamic acid, [4-phenyl-1-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)-4-piperidinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



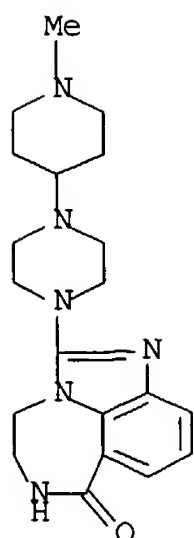
RN 429689-59-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[2-(4-morpholinyl)ethyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)



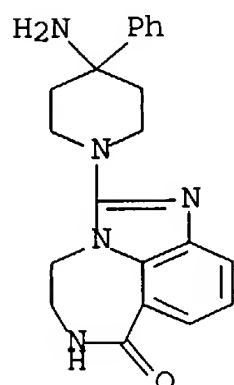
RN 429689-60-1 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(1-methyl-4-piperidinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 429689-61-2 CAPLUS

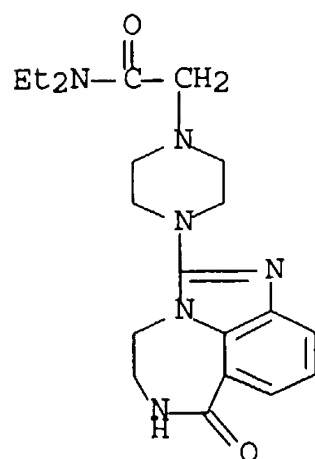
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-amino-4-phenyl-1-piperidinyl)-5,6-dihydro-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

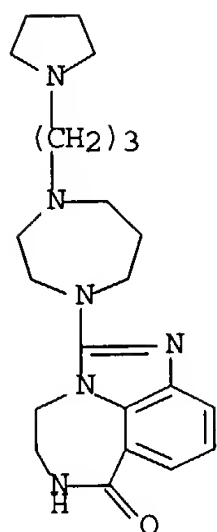
RN 429689-62-3 CAPLUS

CN 1-Piperazineacetamide, N,N-diethyl-4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)

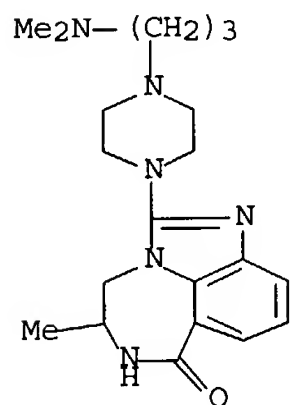


RN 429689-63-4 CAPLUS

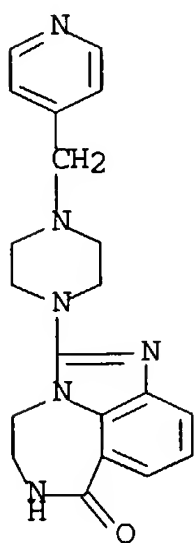
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[hexahydro-4-[3-(1-pyrrolidinyl)propyl]-1H-1,4-diazepin-1-yl]-5,6-dihydro- (9CI) (CA INDEX NAME)



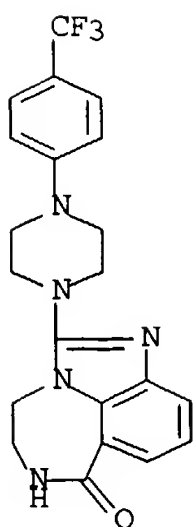
RN 429689-64-5 CAPLUS  
 CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(dimethylamino)propyl]-1-piperazinyl]-5,6-dihydro-5-methyl- (9CI) (CA INDEX NAME)



RN 429689-65-6 CAPLUS  
 CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-pyridinylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



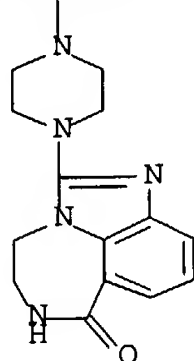
RN 429689-66-7 CAPLUS  
 CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-[4-(trifluoromethyl)phenyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 429689-67-8 CAPLUS

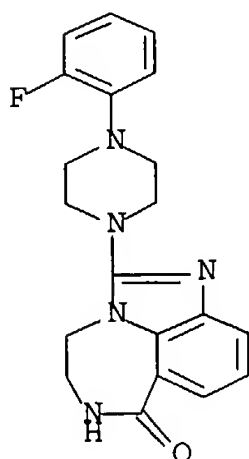
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(3-phenylpropyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

Ph-(CH<sub>2</sub>)<sub>3</sub>



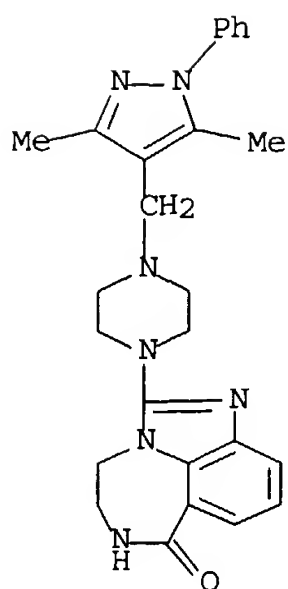
RN 429689-68-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(2-fluorophenyl)-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 429689-69-0 CAPLUS

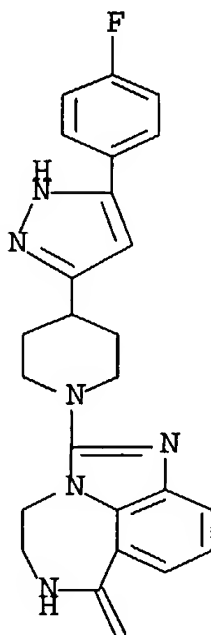
CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[(3,5-dimethyl-1-phenyl-1H-pyrazol-4-yl)methyl]-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



RN 429689-70-3 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[5-(4-fluorophenyl)-1H-pyrazol-3-yl]-1-piperidinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)

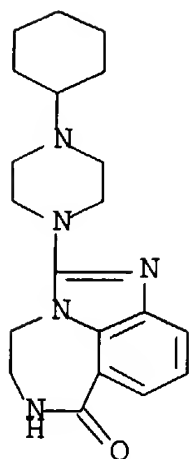
PAGE 1-A



PAGE 2-A

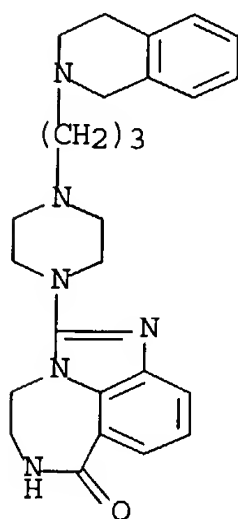
RN 429689-71-4 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-cyclohexyl-1-piperazinyl)-5,6-dihydro- (9CI) (CA INDEX NAME)



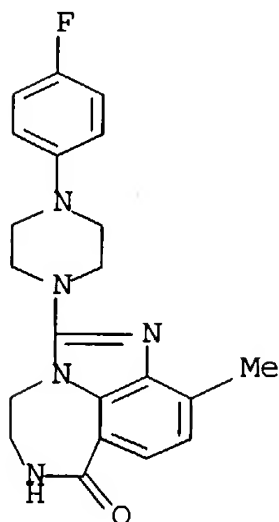
RN 429689-72-5 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-[3-(3,4-dihydro-2(1H)-isoquinolinyl)propyl]-1-piperazinyl]-5,6-dihydro- (9CI) (CA INDEX NAME)



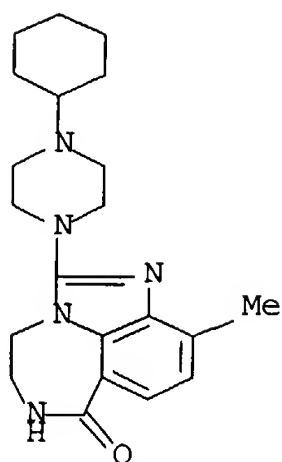
RN 429689-73-6 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-10-methyl- (9CI) (CA INDEX NAME)



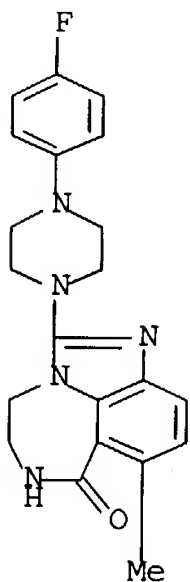
RN 429689-74-7 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-(4-cyclohexyl-1-piperazinyl)-5,6-dihydro-10-methyl- (9CI) (CA INDEX NAME)



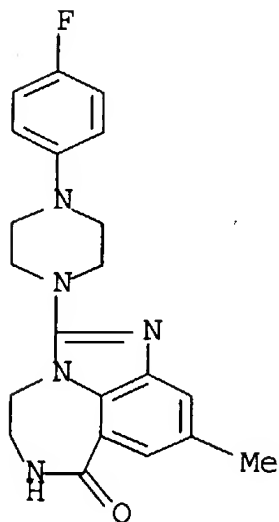
RN 429689-75-8 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-8-methyl- (9CI) (CA INDEX NAME)



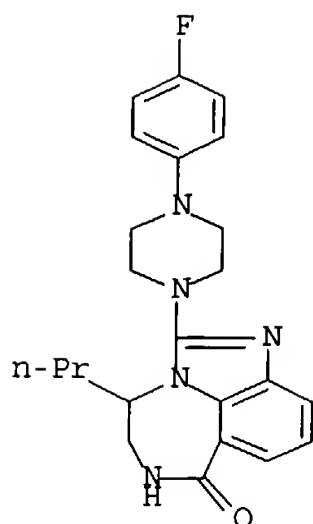
RN 429689-76-9 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-9-methyl- (9CI) (CA INDEX NAME)



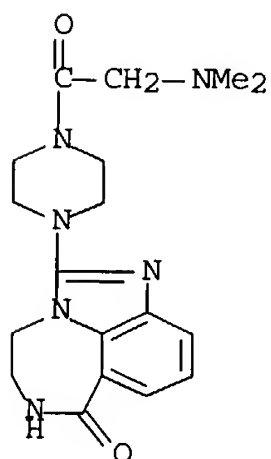
RN 429689-77-0 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 2-[4-(4-fluorophenyl)-1-piperazinyl]-5,6-dihydro-4-propyl- (9CI) (CA INDEX NAME)



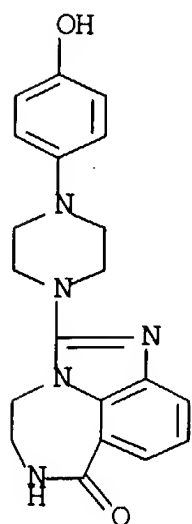
RN 429689-78-1 CAPLUS

CN Piperazine, 1-[(dimethylamino)acetyl]-4-(4,5,6,7-tetrahydro-7-oxoimidazo[4,5,1-jk][1,4]benzodiazepin-2-yl)- (9CI) (CA INDEX NAME)



RN 429689-79-2 CAPLUS

CN Imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one, 5,6-dihydro-2-[4-(4-hydroxyphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



RE.CNT 3

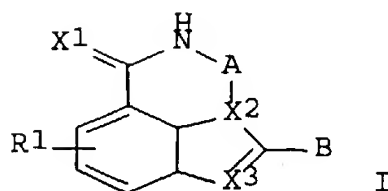
THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 1 OF 2 MARPAT COPYRIGHT 2004 ACS on STN  
 AN 134:266331 MARPAT Full-text  
 TI Preparation of 2-phenyl-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-  
 7(4H)-ones as poly(ADP ribose) polymerase inhibitors.  
 IN Lubisch, Wilfried; Kock, Michael; Hoeger, Thomas; Grandel, Roland;  
 Mueller, Reinhold; Schult, Sabine  
 PA BASF A.-G., Germany  
 SO Ger. Offen., 12 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19946289	A1	20010329	DE 1999-19946289	19990928
	WO 2001023386	A2	20010405	WO 2000-EP9023	20000915
	WO 2001023386	A3	20020510		
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	RW:		GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
	WO 2001023390	A2	20010405	WO 2000-EP9024	20000915
	WO 2001023390	A3	20011227		
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	BR 2000007174	A	20010904	BR 2000-7174	20000915
	EP 1183259	A2	20020306	EP 2000-974379	20000915
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	BR 2000014326	A	20020528	BR 2000-14326	20000915
	EP 1222191	A2	20020717	EP 2000-966022	20000915
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	TR 200101499	T1	20020923	TR 2001-200101499	20000915
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	JP 2003510324	T2	20030318	JP 2001-526538	20000915
	JP 2003510328	T2	20030318	JP 2001-526542	20000915
	ZA 2001004196	A	20020725	ZA 2001-4196	20010523
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	BG 105650	A	20020228	BG 2001-105650	20010626
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	BG 106444	A	20020930	BG 2002-106444	20020226
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PRAI	DE 1999-19946289		19990928		
	DE 2000-10039610		20000809		

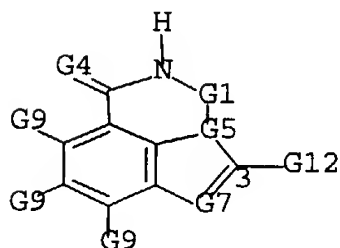
WO 2000-EP9023 20000915  
 WO 2000-EP9024 20000915

GI



AB Title compds. [I; A = (substituted) C1-3 alkylene; X1 = S, O, NE; X2 = N, (substituted) C; X3 = N, CR2; R2 = H, alkyl, alkylphenyl, Ph; R1 = H, halo, OH, NO2, CF3, cyano, alkyl, alkoxy, etc.; B = (unsatd.) (O-, N-, S-interrupted) (substituted) mono-, bi-, tricyclic] were prepared as poly(ADP ribose) polymerase inhibitors (no data). Thus, Me 2-chloro-3-nitrobenzoate was heated with K2CO3 and H2NCH2CH2NH2 in DMF for 3 at 120° to give 9-nitro-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one, which was hydrogenated using Pd/C in EtOH to give 9-amino-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one. The latter in MeOH containing HOAc was treated dropwise with 4-(4-methylpiperazin-1-yl)benzaldehyde in MeOH followed by 1 h stirring at room temperature; Cu(OAc)2, Na2S, and HCl in H2O were added followed by 30 min reflux to give 2-[4-(4-methylpiperazin-1-yl)phenyl]-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one.

MSTR 1



G1 = CH2CH2  
 G4 = O  
 G5 = N  
 G7 = N  
 G12 = piperidino (SO)  
 MPL: claim 1  
 NTE: and tautomers and prodrugs  
 STE: and enantiomers and diastereomers

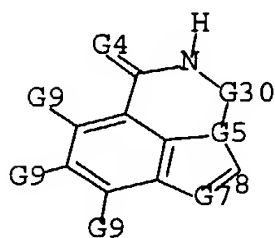
L9 ANSWER 2 OF 2 MARPAT COPYRIGHT 2004 ACS on STN  
 AN 134:261280 MARPAT Full-text  
 TI Azepinoindolone derivatives as poly(ADP-ribose) polymerase inhibitors  
 IN Lubisch, Wilfried; Kock, Michael; Hoeger, Thomas; Grandel, Roland;  
 Mueller, Reinhold; Schult, Sabine  
 PA Basf Aktiengesellschaft, Germany  
 SO PCT Int. Appl., 21 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA German  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2001023390	A2	20010405	WO 2000-EP9024	20000915
	WO 2001023390	A3	20011227		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
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	DE 10039610	A1	20020228	DE 2000-10039610	20000809
	BR 2000007174	A	20010904	BR 2000-7174	20000915
	EP 1183259	A2	20020306	EP 2000-974379	20000915
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
	JP 2003510328	T2	20030318	JP 2001-526542	20000915
	NO 2001002567	A	20010625	NO 2001-2567	20010525
	BG 105650	A	20020228.	BG 2001-105650	20010626
PRAI	DE 1999-19946289		19990928		
	DE 2000-10039610		20000809		
	WO 2000-EP9024		20000915		
AB	Enantiomeric and diastereomeric forms and prodrugs of azepinoindolone derivs. such as 2-(4-(4-n-propylpiperazin-1-yl)phenyl)-1,3,4,5-tetrahydro- 6H-azepino[5,4,3-c,d]indol-6-one are useful as poly(ADP-ribose) polymerase inhibitors. The effectiveness of the title compds. in inhibiting poly(ADP-ribose) polymerase was demonstrated.				

# MSTR 1

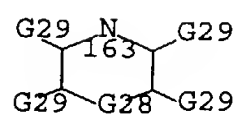
180 G1—G12

G1 = 8

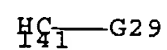


G4 = O  
 G5 = N  
 G7 = N

G12 = 163



G28 = 141



G30 = CH<sub>2</sub>CH<sub>2</sub> (SO)

MPL: claim 1

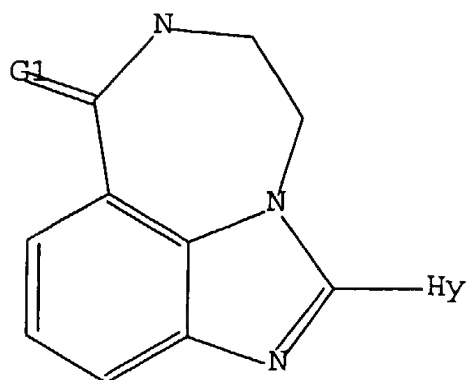
NTE: G5 and G7 are not simultaneously nitrogen

NTE: and tautomers and prodrugs

NTE: substitution is restricted

STE: and enantiomeric and diastereomeric forms

=> d l1; d his; log y  
 L1 HAS NO ANSWERS  
 L1 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

(FILE 'STNGUIDE' ENTERED AT 17:32:57 ON 25 AUG 2004)  
 DEL HIS Y

FILE 'REGISTRY' ENTERED AT 17:35:21 ON 25 AUG 2004  
 L1 STRUCTURE UPLOADED  
 L2 4 S L1  
 L3 38 S L1 FUL

FILE 'CAPLUS' ENTERED AT 17:35:42 ON 25 AUG 2004  
 L4 1 S L3

FILE 'BEILSTEIN' ENTERED AT 17:36:16 ON 25 AUG 2004  
 L5 0 S L1  
 L6 0 S L1 FUL

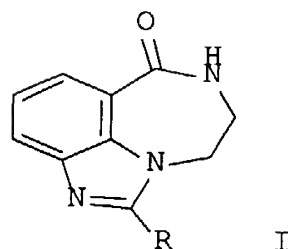
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 L7 0 S L1  
 L8 3 S L1 FUL  
 L9 2 S L8 NOT L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	119.58	964.86
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-1.32	-13.22

STN INTERNATIONAL LOGOFF AT 17:38:57 ON 25 AUG 2004

Chin. 27

L4 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:595169 CAPLUS Full-text  
 DN 140:94018  
 TI Design and synthesis of poly(ADP-ribose) polymerase-1 (PARP-1) inhibitors.  
 part 4: Biological evaluation of imidazobenzodiazepines as potent PARP-1 inhibitors for treatment of ischemic injuries  
 AU Ferraris, Dana; Ficco, Rica Pargas; Dain, David; Ginski, Mark; Lautar, Susan; Lee-Wisdom, Kathy; Liang, Shi; Lin, Qian; Lu, May X.-C.; Morgan, Lisa; Thomas, Bert; Williams, Lawrence R.; Zhang, Jie; Zhou, Yinong; Kalish, Vincent J.  
 CS Guilford Pharmaceuticals Inc., Baltimore, MD, 21224, USA  
 SO Bioorganic & Medicinal Chemistry (2003), 11(17), 3695-3707  
 CODEN: BMECEP; ISSN: 0968-0896  
 PB Elsevier Science Ltd.  
 DT Journal  
 LA English  
 OS CASREACT 140:94018  
 GI

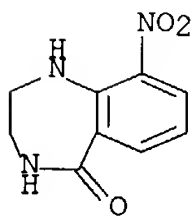


AB Imidazobenzodiazepines such as I [R = PhCH<sub>2</sub>CH<sub>2</sub>, 4-Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>] are prepared as poly(ADP-ribose) polymerase (PARP-1) inhibitors for the treatment of ischemic injury and diabetes mellitus. Addition of ionizable groups (such as dialkylaminomethyl substituents at the 2-position of imidazobenzodiazepines) improved the pharmaceutical characteristics of the imidazobenzodiazepines while affecting their inhibition of PARP-1 only slightly. Mol. modeling of the inhibitors in the active site of PARP-1, structure-activity relationships of imidazobenzodiazepines for PARP-1 inhibition, and the pharmacokinetics of selected imidazobenzodiazepines are discussed. Administration of compds. such as I [R = 4-Me<sub>2</sub>N(CH<sub>2</sub>)<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>] to mice with streptozotocin-induced diabetes results in maintenance of glucose levels. I (R = PhCH<sub>2</sub>CH<sub>2</sub>) (IC<sub>50</sub> = 26 nM) reduces infarct volume in the rat model of permanent focal cerebral ischemia.

IT **328546-65-2P 328546-66-3P**  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation, structure-active relationships, and pharmacokinetics of imidazobenzodiazepine inhibitors of poly(ADP-ribose) polymerase-1 as potential antidiabetic and antiischemic agents)

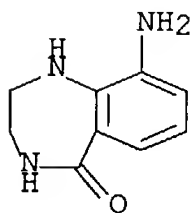
RN 328546-65-2 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



RN 328546-66-3 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



IT 433728-54-2P 433728-59-7P 433728-60-0P

433728-61-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

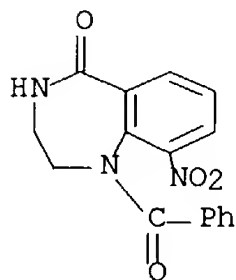
RACT

(Reactant or reagent)

(preparation, structure-active relationships, and pharmacokinetics of imidazobenzodiazepine inhibitors of poly(ADP-ribose) polymerase-1 as potential antidiabetic and antiischemic agents)

RN 433728-54-2 CAPLUS

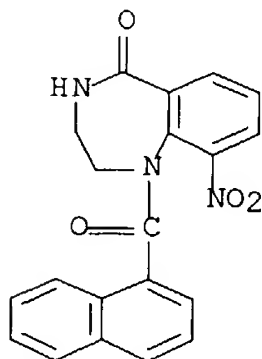
CN 5H-1,4-Benzodiazepin-5-one, 1-benzoyl-1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



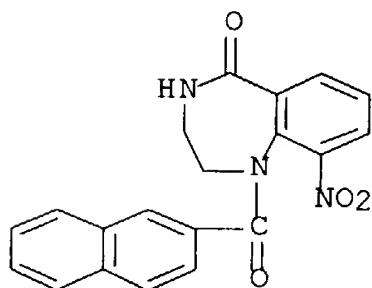
RN 433728-59-7 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-1-(1-

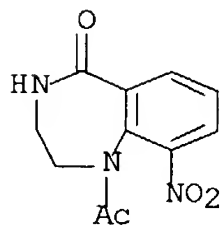
naphthalenylcarbonyl)-  
9-nitro- (9CI) (CA INDEX NAME)



RN 433728-60-0 CAPLUS  
CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-1-(2-naphthalenylcarbonyl)-  
9-nitro- (9CI) (CA INDEX NAME)

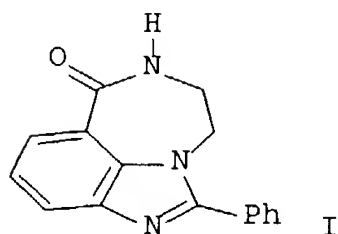


RN 433728-61-1 CAPLUS  
CN 5H-1,4-Benzodiazepin-5-one, 1-acetyl-1,2,3,4-tetrahydro-9-nitro- (9CI)  
(CA INDEX NAME)

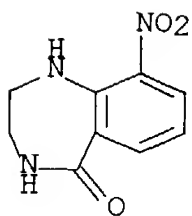


RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2002:954525 CAPLUS Full-text  
 DN 138:170205  
 TI Tricyclic Benzimidazoles as Potent Poly(ADP-ribose) Polymerase-1 Inhibitors  
 AU Skalitzky, Donald J.; Marakovits, Joseph T.; Maegley, Karen A.; Ekker, Anne; Yu, Xiao-Hong; Hostomsky, Zdenek; Webber, Stephen E.; Eastman, Brian  
 W.; Almassy, Robert; Li, Jianke; Curtin, Nicola J.; Newell, David R.; Calvert, A. Hilary; Griffin, Roger J.; Golding, Bernard T.  
 CS Pfizer Global R&D, La Jolla/Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA  
 SO Journal of Medicinal Chemistry (2003), 46(2), 210-213  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 138:170205  
 GI



AB Novel tricyclic benzimidazole carboxamide poly(ADP-ribose) polymerase-1 (PARP-1) inhibitors, e.g., I, have been synthesized. Several compds. were found to be powerful chemopotentiators of temozolomide and topotecan in both A549 and LoVo cell lines. In vitro inhibition of PARP-1 was confirmed by direct measurement of NAD<sup>+</sup> depletion and ADP-ribose polymer formation caused by chemical induced DNA damage.  
 IT **328546-65-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (first attempted preparation of intermediate aminobenzodiazepinone via addition  
 of acrylonitrile to o-nitroaniline with subsequent hydrolysis, cyclization and nitrogen insertion via Schmidt reaction)  
 RN 328546-65-2 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



IT **328546-66-3P**

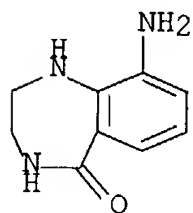
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT

(Reactant or reagent)

(preparation of intermediate aminobenzodiazepinone via cyclization of  
 nitrobromobenzoic acid Me ester with ethylene diamine and subsequent  
 reduction)

RN 328546-66-3 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro- (9CI) (CA INDEX  
 NAME)



RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:428911 CAPLUS Full-text

DN 137:6205

TI Preparation of benzazepinones, isoquinolinones and related compounds as inhibitors of poly(ADP-ribose) polymerase (PARP) for the prevention and/or

treatment of tissue damage from cell trauma or cell death due to necrosis

or apoptosis.

IN Ferraris, Dana V.; Li, Jia-He; Kalish, Vincent J.; Zhang, Jie

PA Guilford Pharmaceuticals Inc., USA

SO PCT Int. Appl., 152 pp.

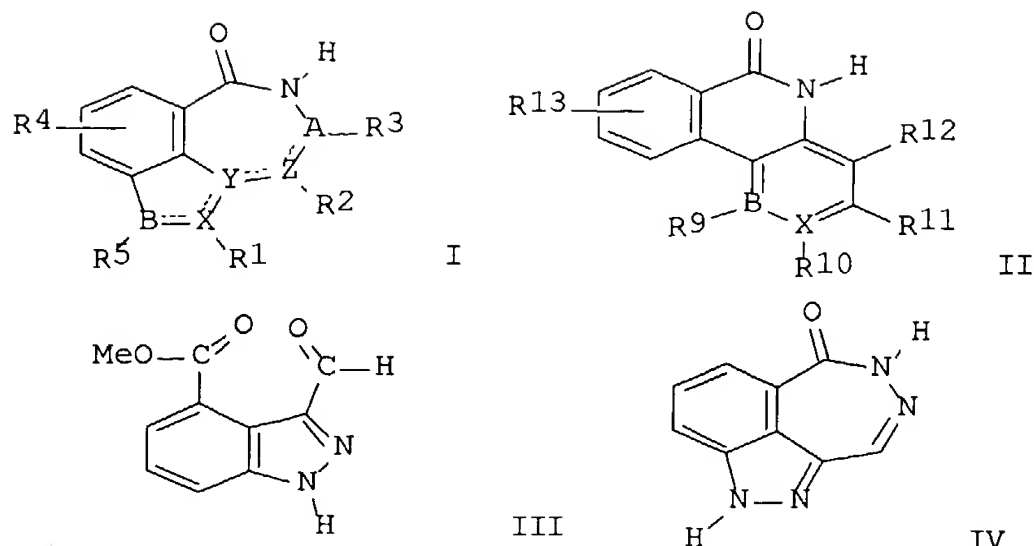
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	WO 2002044183	A2	20020606	WO 2001-US44815	20011130
	WO 2002044183	A3	20030522		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2002036521	A5	20020611	AU 2002-36521	20011130
	US 2003022883	A1	20030130	US 2001-996776	20011130
	EP 1339402	A2	20030903	EP 2001-986053	20011130
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
	JP 2004517831	T2	20040617	JP 2002-546553	20011130
PRAI	US 2000-250132P	P	20001201		
	US 2001-310274P	P	20010809		
	WO 2001-US44815	W	20011130		
OS	MARPAT 137:6205				
GI					



AB This invention discloses the preparation of title compds. I and II, their pharmaceutically acceptable salts, and related compds. as inhibitors of poly(ADP-ribose) polymerase (PARP) [wherein: A = N, C, CH<sub>2</sub>, CH; B = C, N, NH, S, SO, SO<sub>2</sub>; X = C, CH, N; Y = C, N; Z = C, CH<sub>2</sub>, N, CO; provided that at least one of X, Y, or Z is N; R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>5</sub> when present are optionally or independently = H, OH, :O, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, halogen, amine, COR<sub>8</sub> (R<sub>8</sub> = H, OH, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl), OR<sub>6</sub>, NR<sub>6</sub>R<sub>7</sub> (R<sub>6</sub>, R<sub>7</sub> independently = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl); R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>5</sub> optionally form ring through a straight or branched C1-4alkyl which may addnl. contain 1-2 double or triple bonds; R<sub>4</sub> = 1-3 of H, halo, or alkyl; with proviso that when A, X, or Z = C, then R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub> when present may also independently = halogen, CN, O; R<sub>9</sub>, R<sub>10</sub>, R<sub>11</sub>, R<sub>12</sub> optionally or independently = H, halogen, amino, OH, halo-amine, O-alkyl, O-aryl, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, carboxy, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, COR<sub>8</sub>; R<sub>13</sub> = 1-3 of H, halogen, alkoxy, alkyl]. For example, cyclocondensation of formylindazole III (prepared from Me indole-4-carboxylate and NaNO<sub>2</sub>/AcOH), with hydrazine provided claimed benzoazulenone IV as a white solid. Benzoazulenone IV inhibited human recombinant PARP at an IC<sub>50</sub> of 0.018 μM. PARP IC<sub>50</sub> inhibition studies for an addnl. 156 examples are provided, ranging in values from 0.01 to 20 μM. Biol. data are provided for the in vivo treatment of focal cerebral ischemia and gout via PARP inhibition with selected compds. II. The present invention is believed to protect cells, tissue and organs against the ill-effects of reactive free radicals and nitric oxide through inhibition of PARP activity.

IT **328546-65-2P 328546-66-3P 433728-54-2P**  
**433728-55-3P 433728-56-4P 433728-57-5P**  
**433728-58-6P 433728-59-7P 433728-60-0P**  
**433728-61-1P**

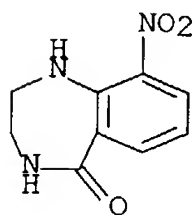
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT  
 (Reactant or reagent)  
 (intermediate; preparation of benzazepinones, isoquinolinones and

related

compds. as inhibitors of poly(ADP-ribose) polymerase (PARP))

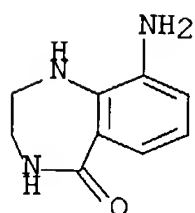
RN 328546-65-2 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



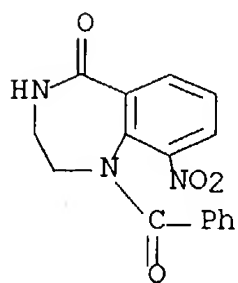
RN 328546-66-3 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



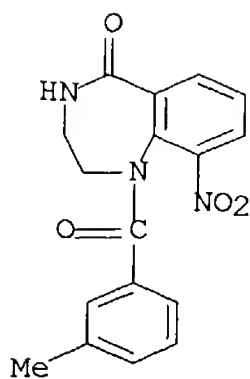
RN 433728-54-2 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1-benzoyl-1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)

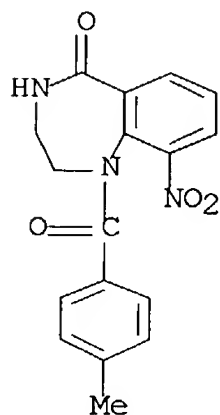


RN 433728-55-3 CAPLUS

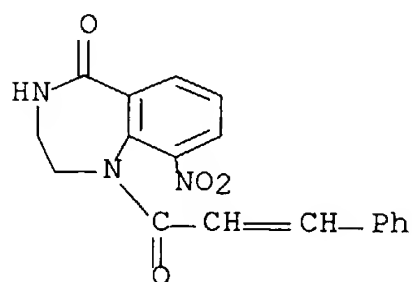
CN 5H-1,4-Benzodiazepin-5-one, 1-(3-methylbenzoyl)-9-nitro- (9CI) (CA INDEX NAME)



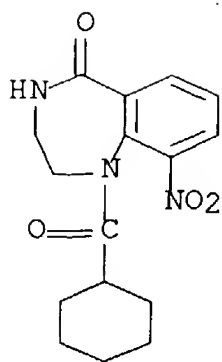
RN 433728-56-4 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-1-(4-methylbenzoyl)-9-nitro-  
 (9CI) (CA INDEX NAME)



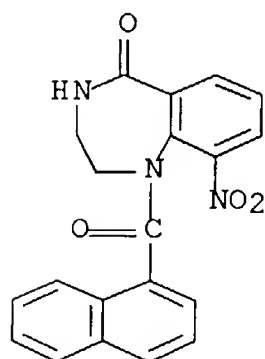
RN 433728-57-5 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro-1-(1-oxo-3-phenyl-2-propenyl)-  
 (9CI) (CA INDEX NAME)



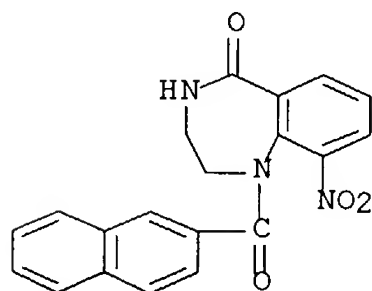
RN 433728-58-6 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1-(cyclohexylcarbonyl)-1,2,3,4-tetrahydro-9-nitro-  
 (9CI) (CA INDEX NAME)



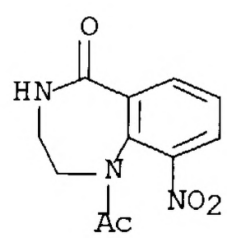
RN 433728-59-7 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-1-(1-naphthalenylcarbonyl)-  
 9-nitro- (9CI) (CA INDEX NAME)



RN 433728-60-0 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-1-(2-naphthalenylcarbonyl)-  
 9-nitro- (9CI) (CA INDEX NAME)



RN 433728-61-1 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1-acetyl-1,2,3,4-tetrahydro-9-nitro- (9CI)  
 (CA INDEX NAME)

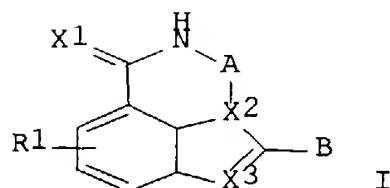


L4 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:225212 CAPLUS Full-text  
 DN 134:266331  
 TI Preparation of 2-phenyl-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-  
 7(4H)-ones as poly(ADP ribose) polymerase inhibitors.  
 IN Lubisch, Wilfried; Kock, Michael; Hoeger, Thomas; Grandel, Roland;  
 Mueller, Reinhold; Schult, Sabine  
 PA BASF A.-G., Germany  
 SO Ger. Offen., 12 pp.  
 CODEN: GWXXBX  
 DT Patent  
 LA German  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19946289	A1	20010329	DE 1999-19946289	19990928
	WO 2001023386	A2	20010405	WO 2000-EP9023	20000915
	WO 2001023386	A3	20020510		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	WO 2001023390	A2	20010405	WO 2000-EP9024	20000915
	WO 2001023390	A3	20011227		
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	BR 2000007174	A	20010904	BR 2000-7174	20000915
	EP 1183259	A2	20020306	EP 2000-974379	20000915
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000014326	A	20020528	BR 2000-14326	20000915
	EP 1222191	A2	20020717	EP 2000-966022	20000915
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	TR 200101499	T1	20020923	TR 2001-200101499	20000915
	TR 200200820	T2	20020923	TR 2002-200200820	20000915
	JP 2003510324	T2	20030318	JP 2001-526538	20000915
	JP 2003510328	T2	20030318	JP 2001-526542	20000915
	ZA 2001004196	A	20020725	ZA 2001-4196	20010523
	NO 2001002567	A	20010625	NO 2001-2567	20010525
	BG 105650	A	20020228	BG 2001-105650	20010626
	ZA 2002001494	A	20031003	ZA 2002-1494	20020222
	BG 106444	A	20020930	BG 2002-106444	20020226
	NO 2002001379	A	20020320	NO 2002-1379	20020320
PRAI	DE 1999-19946289	A	19990928		

DE 2000-10039610	A	20000809
WO 2000-EP9023	W	20000915
WO 2000-EP9024	W	20000915

OS MARPAT 134:266331  
GI



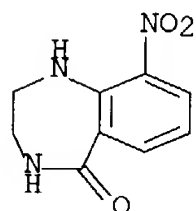
AB Title compds. [I; A = (substituted) C1-3 alkylene; X1 = S, O, NE; X2 = N, (substituted) C; X3 = N, CR2; R2 = H, alkyl, alkylphenyl, Ph; R1 = H, halo, OH, NO2, CF3, cyano, alkyl, alkoxy, etc.; B = (unsatd.) (O-, N-, S-interrupted) (substituted) mono-, bi-, tricyclic] were prepared as poly(ADP ribose) polymerase inhibitors (no data). Thus, Me 2-chloro-3-nitrobenzoate was heated with K2CO3 and H2NCH2CH2NH2 in DMF for 3 at 120° to give 9-nitro-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one, which was hydrogenated using Pd/C in EtOH to give 9-amino-1,2,3,4-tetrahydro-5H-1,4-benzodiazepin-5-one. The latter in MeOH containing HOAc was treated dropwise with 4-(4-methylpiperazin-1-yl)benzaldehyde in MeOH followed by 1 h stirring at room temperature; Cu(OAc)2, Na2S, and HCl in H2O were added followed by 30 min reflux to give 2-[4-(4-methylpiperazin-1-yl)phenyl]-5,6-dihydro-imidazo[4,5,1-jk][1,4]benzodiazepin-7(4H)-one.

IT **328546-65-2P 328546-66-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of phenyldihydroimidazobenzodiazepinones as PARP inhibitors)

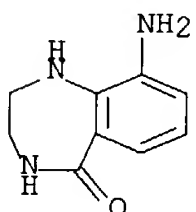
RN 328546-65-2 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



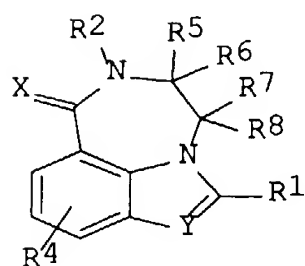
RN 328546-66-3 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:167995 CAPLUS Full-text  
 DN 134:207833  
 TI Preparation of tricyclic inhibitors of poly(ADP-ribose) polymerases  
 IN Webber, Stephen Evan; Skaltitzky, Donald James; Tikhe, Jayashree Girish;  
 Kumpf, Robert Arnold; Marakovits, Joseph Timothy; Eastman, Walter Brian  
 PA Agouron Pharmaceuticals, Inc., USA; Cancer Research Campaign Technology  
 Limited  
 SO PCT Int. Appl., 236 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001016136	A2	20010308	WO 2000-US23882	20000831
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	EP 1208104	A2	20020529	EP 2000-961437	20000831
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
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	JP 2003513015	T2	20030408	JP 2001-519702	20000831
	US 6548494	B1	20030415	US 2000-653184	20000831
	EE 200200100	A	20030616	EE 2002-100	20000831
	NZ 516793	A	20040326	NZ 2000-516793	20000831
	NO 2002000421	A	20020425	NO 2002-421	20020128
	ZA 2002000830	A	20030130	ZA 2002-830	20020130
	BG 106562	A	20030331	BG 2002-106562	20020329
PRAI	US 1999-152142P	P	19990831		
	WO 2000-US23882	W	20000831		
OS	MARPAT 134:207833				
GI					



I

AB The title compds. [I; X = O, S; Y = N, CR3 (wherein R3 = halo, CN, alkyl, etc.); R1 = H, halo, CN, etc.; R2 = H, alkyl; R4 = H, halo, alkyl; R5-R8 = H, alkyl, alkenyl, aryl, etc.] which are poly(ADP-ribosyl)transferase inhibitors, and are useful in treating cancers and in ameliorating the effects of stroke, head trauma, and neurodegenerative disease, were prepared E.g., a multi-step synthesis of 1-phenyl-8,9-dihydro-7H-2,7,9a-triaza- benzo[cd]azulen-6-one [I; Y = N; X = O; R1 = Ph; R2, R4-R8 = H] was given. Biol. data for compds. I were presented.

IT **328546-65-2P 328546-66-3P 328546-74-3P**  
**328546-75-4P 328546-88-9P 328547-02-0P**  
**328547-14-4P 328547-18-8P 328547-19-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

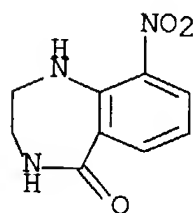
RACT

(Reactant or reagent)

(preparation of tricyclic inhibitors of poly(ADP-ribose) polymerases)

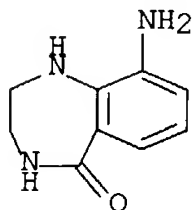
RN 328546-65-2 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



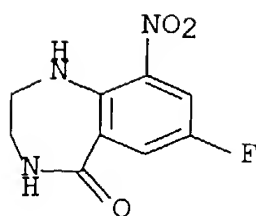
RN 328546-66-3 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

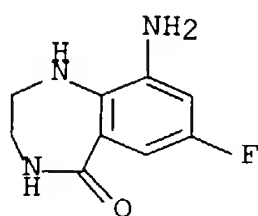


RN 328546-74-3 CAPLUS

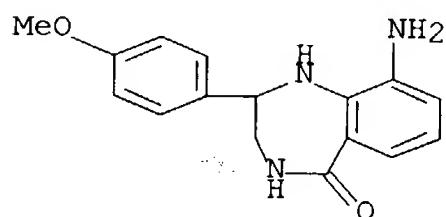
CN 5H-1,4-Benzodiazepin-5-one, 7-fluoro-1,2,3,4-tetrahydro-9-nitro- (9CI) (CA INDEX NAME)



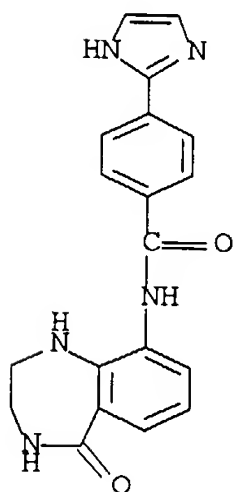
RN 328546-75-4 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 9-amino-7-fluoro-1,2,3,4-tetrahydro- (9CI)  
 (CA INDEX NAME)



RN 328546-88-9 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

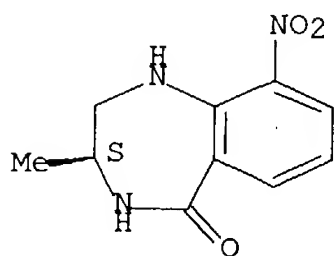


RN 328547-02-0 CAPLUS  
 CN Benzamide, 4-(1H-imidazol-2-yl)-N-(2,3,4,5-tetrahydro-5-oxo-1H-1,4-benzodiazepin-9-yl)- (9CI) (CA INDEX NAME)



RN 328547-14-4 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro-, (3S)- (9CI) (CA INDEX NAME)

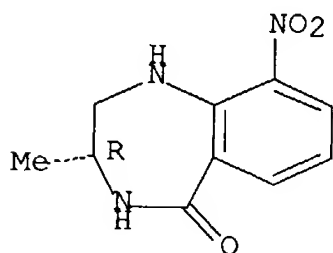
Absolute stereochemistry.



RN 328547-18-8 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro-, (3R)-  
(9CI) (CA INDEX NAME)

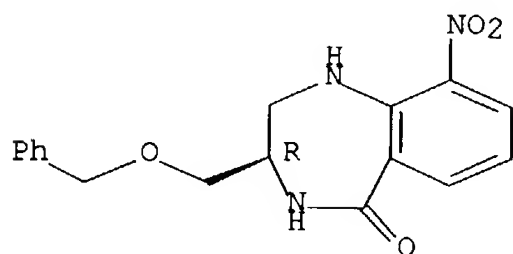
Absolute stereochemistry.



RN 328547-19-9 CAPLUS

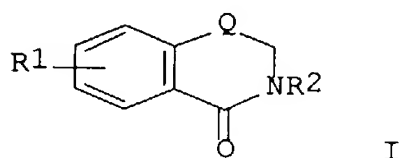
CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-9-nitro-3-  
[(phenylmethoxy)methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1996:117830 CAPLUS Full-text  
 DN 124:176144  
 TI Preparation of bicyclic compds. as antirheumatics  
 IN Kawagoe, Keiichi; Nakayama, Atsushi; Hasegawa, Masashi; Miwa, Tamotsu;  
 Nakajima, Hiroto; Tsukada, Hisashi  
 PA Daiichi Seiyaku Co, Japan  
 SO Jpn. Kokai Tokkyo Koho, 24 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 07258224	A2	19951009	JP 1994-53359	19940324
PRAI	JP 1994-53359		19940324		
OS	MARPAT 124:176144				
GI					



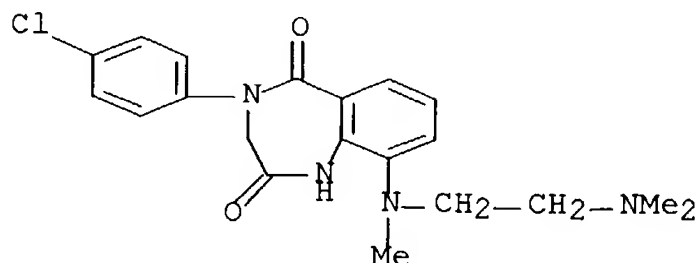
AB Bicyclic compds. I [R1 = H, amino, substituted amino, nitrogen-containing heterocyclyl, substituted nitrogen-containing heterocyclyl; R2 = aryl, substituted aryl; Q = N:CR3, NHCR4R5, NHCO(CH2)n; R3 = H, alkyl, substituted alkyl; R4, R5 = H, alkyl; n = 1, 2] and their salts, useful as antirheumatics, immunosuppressants, allergy inhibitors, and for treatment for bone disease, were prepared. Thus, stirring 2-amino-N-(4-chlorophenyl)-3-(4-methylpiperazino)benzamide with tri-Et orthoformate and a catalytic amount of H2SO4 at 110° for 5 h gave 92% 3-(4-chlorophenyl)-8-(4-methylpiperazino)-3,4-dihydroquinazolin-4-one. 3-(4-Chlorophenyl)-2-methyl-8-(4-methylpiperazino)-3,4-dihydroquinazolin-4-one showed antiinflammatory activity in rats.

IT **173589-72-5P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of bicyclic compds. as antirheumatics)

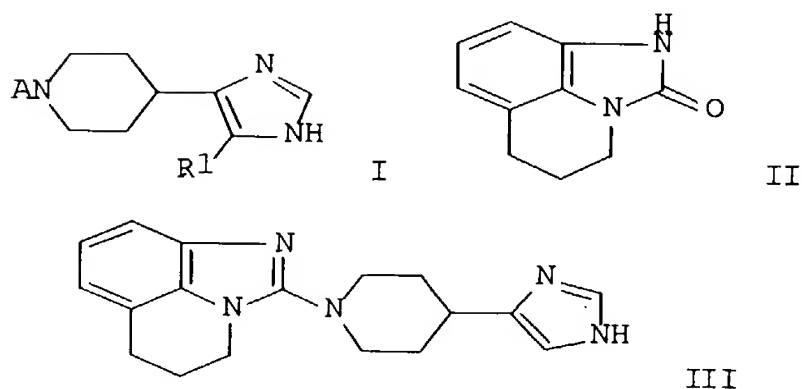
RN 173589-72-5 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 4-(4-chlorophenyl)-9-[[2-(dimethylamino)ethyl]methylamino]-3,4-dihydro- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:557370 CAPLUS Full-text  
 DN 122:290862  
 TI Derivatives of imidazol-4-ylpiperidine with 5-HT3 and 5-HT4 activity,  
 their preparation, and their use in therapy.  
 IN Jegham, Samir; Defosse, Gerard; Purcell, Thomas Andrew; Even, Luc  
 PA Synthelabo S. A., Fr.  
 SO Eur. Pat. Appl., 17 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA French  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 646583	A1	19950405	EP 1994-402114	19940923
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT,				
SE	FR 2710915	A1	19950414	FR 1993-11771	19931004
	FR 2710915	B1	19951124		
	CA 2133491	AA	19950405	CA 1994-2133491	19941003
	NO 9403682	A	19950405	NO 1994-3682	19941003
	FI 9404600	A	19950405	FI 1994-4600	19941003
	AU 9474329	A1	19950413	AU 1994-74329	19941003
	JP 07179466	A2	19950718	JP 1994-238914	19941003
	ZA 9407710	A	19950810	ZA 1994-7710	19941003
	CN 1109471	A	19951004	CN 1994-117012	19941003
	HU 71120	A2	19951128	HU 1994-2832	19941003
	US 5589476	A	19961231	US 1994-317661	19941003
PRAI	FR 1993-11771		19931004		
OS	CASREACT 122:290862; MARPAT 122:290862				
GI					



AB Title compds. I [R1 = H, straight or branched C1-6 alkyl; A = 9 specific tricyclic heterocyclic radicals with an optional phenylmethyl substituent] and their pharmaceutical salts are claimed. The compds. are ligands of 5-HT3 and 5-HT4 receptors, and have a variety of potential uses involving CNS and cardiovascular activities. For example, reduction of 8-quinolinamine with Na in EtOH gave the 1,2,3,4-

tetrahydro derivative, which was cyclized with urea to give dihydroimidazoquinolinone II. Treatment of II with POCl<sub>3</sub> converted the carbonyl to the corresponding unsatd. chloride, which reacted with 4-(1H-imidazol-4-yl)piperidine in isoamyl alc. at 120° to give title compound III. The IC<sub>50</sub> values of more active I for inhibition of [3H]-quipazine binding to rat cerebral 5-HT<sub>3</sub> receptors were 0.01-10 nM. I also had IC<sub>50</sub> of 0.02-2 μM for inhibition of specific binding of [3H]-GR118808 to guinea pig 5-HT<sub>4</sub> receptors.

IT **126234-17-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT

(Reactant or reagent)

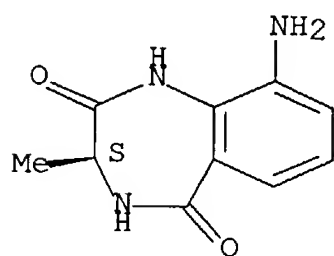
(intermediate; preparation of imidazolylpiperidine derivs. as 5-HT<sub>3</sub>  
 and 5-HT<sub>4</sub> receptor ligands)

RN 126234-17-1 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)-  
 (9CI)

(CA INDEX NAME)

Absolute stereochemistry.



IT **131645-80-2**

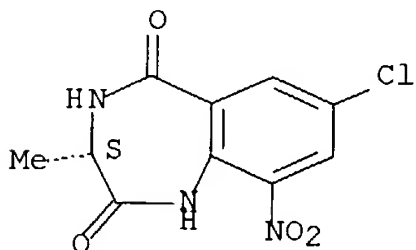
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of imidazolylpiperidine derivs. as 5-HT<sub>3</sub> and 5-HT<sub>4</sub> receptor ligands)

RN 131645-80-2 CAPLUS

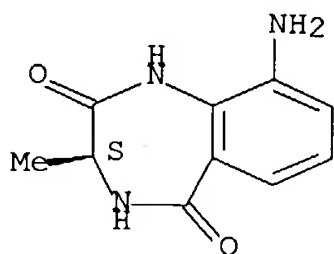
CN 1H-1,4-Benzodiazepine-2,5-dione, 7-chloro-3,4-dihydro-3-methyl-9-nitro-,  
 (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

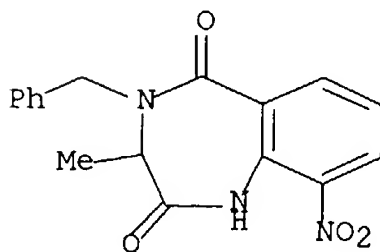


L4 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:502782 CAPLUS Full-text  
 DN 123:112027  
 TI Synthesis of racemic and enantiomeric (S)-(+)-4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one derivatives  
 AU Pfaendler, Hans Rudolf; Weisner, Frank  
 CS Inst. Organic Chem., Univ. Munich, Munich, D-80333, Germany  
 SO Heterocycles (1995), 40(2), 717-27  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PB Japan Institute of Heterocyclic Chemistry  
 DT Journal  
 LA English  
 OS CASREACT 123:112027  
 AB Racemic and enantiomeric (S)-(+)-4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one derivs. were prepared using free amino acids and 3-nitroisatoic anhydride. Simultaneous reduction of two amide functions was efficiently achieved using diborane.  
 IT **126234-17-1P 166044-60-6P 166044-61-7P 166044-62-8P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT  
 (Reactant or reagent)  
 (synthesis of racemic and enantiomeric tetrahydromethylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one derivs.)  
 RN 126234-17-1 CAPLUS  
 CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)- (9CI)  
 (CA INDEX NAME)

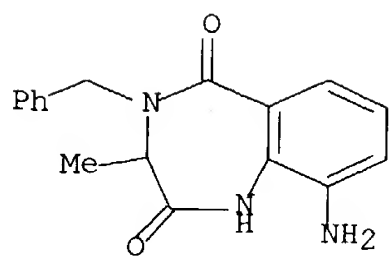
Absolute stereochemistry.



RN 166044-60-6 CAPLUS  
 CN 1H-1,4-Benzodiazepine-2,5-dione, 3,4-dihydro-3-methyl-9-nitro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 166044-61-7 CAPLUS  
 CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

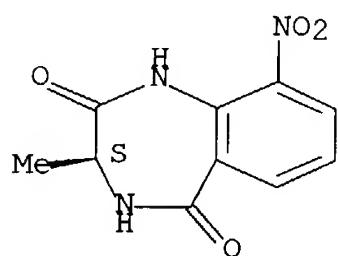


RN 166044-62-8 CAPLUS

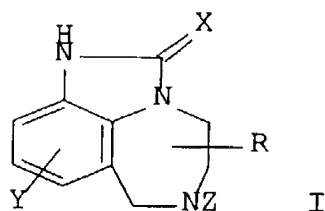
CN 1H-1,4-Benzodiazepine-2,5-dione, 3,4-dihydro-3-methyl-9-nitro-, (S)-  
(9CI)

(CA INDEX NAME)

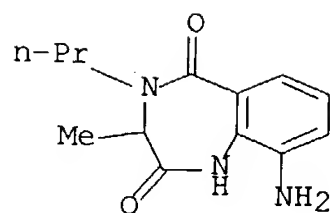
Absolute stereochemistry.



L4 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:380741 CAPLUS Full-text  
 DN 122:290829  
 TI Synthesis and Anti-HIV-1 Activity of 4,5,6,7-Tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) Derivatives.  
 3  
 AU Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; Miranda, Milton; Rodgers, James D.; Hitchens, T. Kevin; Leo, Gregory; et al.  
 CS Janssen Research Foundation, Spring House, PA, 19477, USA  
 SO Journal of Medicinal Chemistry (1995), 38(5), 771-93  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PB American Chemical Society  
 DT Journal  
 LA English  
 GI



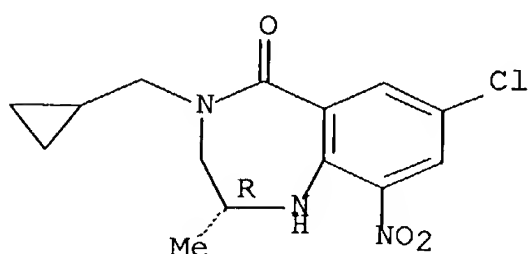
AB 4,5,6,7-Tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-ones (TIBO) (I, R = H, 5-Et, 7-Ph, etc.; X = S, O; Y = 8-Cl, 9-Cl; Z = H, 3,3-dimethylallyl, Pr, etc.) have been shown to significantly inhibit HIV-1 replication in vitro by interfering with the virus's reverse transcriptase enzyme. We describe our synthetic endeavors around 4, 5, and 7 mono- and disubstitutions of I and discuss HIV-1 inhibitory structure-activity relationships. On the basis of inhibition of HIV-1 replication in MT-4 cells, we found that 5-mono-Me-substituted analogs and 7-mono-Me-substituted analogs of I were comparable as being consistently the most active compds. Although generally less active, the 4,5,7-unsubstituted, 4-mono-substituted, cis- and trans-5,7-di-Me-substituted, and cis-4,5-di-Me-substituted analogs of I also exhibited significant activity. The remaining trans-4,5-di-Me-substituted, cis- and trans-4,7-di-Me-substituted, and all 4,5-, 5,6-, 6,7-, and 7,8-fused disubstituted analogs of I possessed no noticeable desired activity.  
 IT **131645-75-5P 162930-68-9P 162930-69-0P**  
**162930-71-4P 162930-72-5P 162931-22-8P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
 (synthesis and anti-HIV-1 activity of imidazobenzodiazepinones)  
 RN 131645-75-5 CAPLUS  
 CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-4-propyl-(9CI) (CA INDEX NAME)



RN 162930-68-9 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 7-chloro-4-(cyclopropylmethyl)-1,2,3,4-tetrahydro-2-methyl-9-nitro-, (R)- (9CI) (CA INDEX NAME)

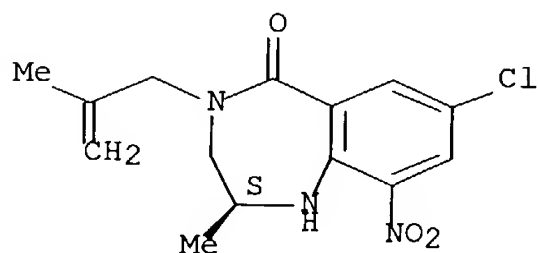
Absolute stereochemistry.



RN 162930-69-0 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 7-chloro-1,2,3,4-tetrahydro-2-methyl-4-(2-methyl-2-propenyl)-9-nitro-, (S)- (9CI) (CA INDEX NAME)

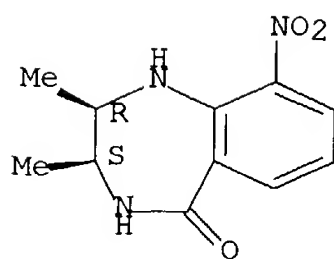
Absolute stereochemistry.



RN 162930-71-4 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-2,3-dimethyl-9-nitro-, cis- (9CI) (CA INDEX NAME)

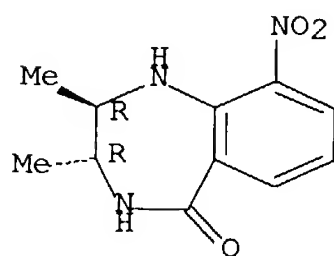
Relative stereochemistry.



RN 162930-72-5 CAPLUS

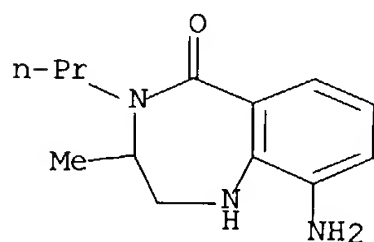
CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-2,3-dimethyl-9-nitro-,  
trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 162931-22-8 CAPLUS

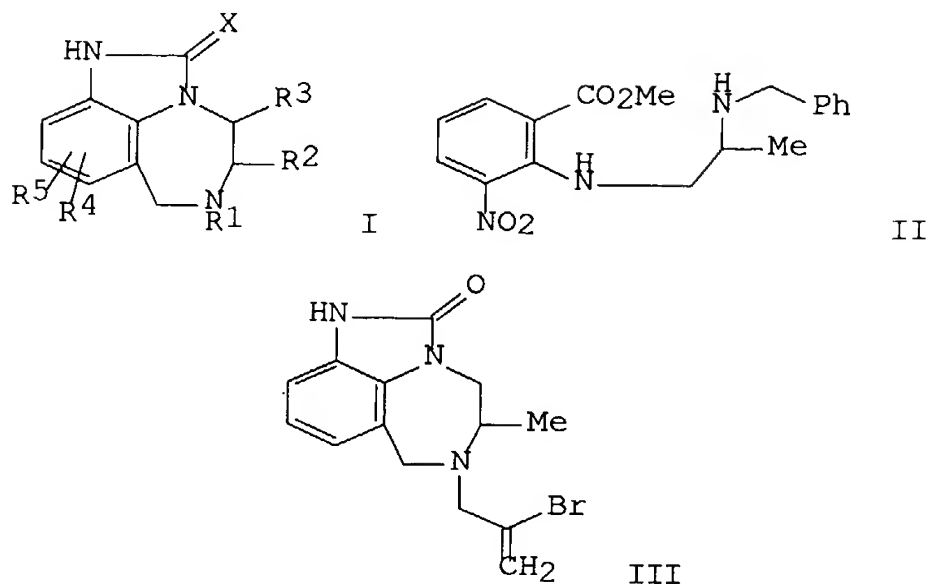
CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-3-methyl-4-  
propyl-  
(9CI) (CA INDEX NAME)



L4 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1992:235663 CAPLUS Full-text  
 DN 116:235663  
 TI Preparation of antiviral tetrahydroimidazo[1,4]benzodiazepin-2-(thio)ones  
 IN Kukla, Michael Joseph; Breslin, Henry Joseph; Raeymaekers, Alfons Herman  
 Margaretha; Van Gelder, Josephus Ludovicus Hubertus; Janssen, Paul  
 Adriaan  
 Jan  
 PA Janssen Pharmaceutica N. V., Belg.  
 SO PCT Int. Appl., 48 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9200979	A1	19920123	WO 1991-EP1224	19910628
	W: AU, BB, BG, BR, CA, FI, HU, JP, KP, KR, LK, MC, MG, MW, NO, PL, RO, SD, SU				
	RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	CA 2086547	AA	19920107	CA 1991-2086547	19910628
	AU 9180683	A1	19920204	AU 1991-80683	19910628
	AU 644192	B2	19931202		
	EP 538297	A1	19930428	EP 1991-912145	19910628
	EP 538297	B1	20010919		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 05508632	T2	19931202	JP 1991-511094	19910628
	HU 68382	A2	19950628	HU 1993-11	19910628
	PL 168320	B1	19960229	PL 1991-297379	19910628
	PL 169662	B1	19960830	PL 1991-309617	19910628
	PL 169613	B1	19960830	PL 1991-309618	19910628
	AT 205848	E	20011015	AT 1991-912145	19910628
	ES 2164044	T3	20020216	ES 1991-912145	19910628
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	SK 278442	B6	19970507	SK 1991-2065	19910704
	ZA 9105239	A	19930331	ZA 1991-5239	19910705
	CN 1057840	A	19920115	CN 1991-104581	19910706
	CN 1034122	B	19970226		
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	US 5270464	A	19931214	US 1993-42858	19930405
	US 5371079	A	19941206	US 1993-132030	19931005
	US 6201119	B1	20010313	US 1994-304951	19941017
PRAI	US 1990-549349	A	19900706		
	GB 1988-6449	A	19880318		
	GB 1989-4108	A	19890223		
	US 1989-323585	B2	19890314		
	GB 1989-20354	A	19890908		
	US 1989-406625	B2	19890913		
	US 1989-406626	B2	19890913		
	US 1990-476926	B2	19900208		
	US 1990-549777	B2	19900709		
	US 1990-583533	B2	19900917		
	US 1991-671238	B1	19910319		
	WO 1991-EP1224	A	19910628		

US 1993-42858 A3 19930405  
 US 1993-132030 A3 19931005  
 OS MARPAT 116:235663  
 GI



AB Title compds. [I; X = O, S; R1 = (substituted) alkenyl, cycloalkylalkyl, alkylthioalkyl, alkylsulfinylalkyl, alkylsulfonylalkyl, etc.; R2, R3 = H, alkyl; R4, R5 = H, alkyl, halo, cyano, NO2, CF3, OH, alkoxy, (alkyl)amino, alkylcarbonylamino, arylcarbonylamino], were prepared Thus, diamine II [preparation from Me 2-bromo-3-nitrobenzoate and (H2NCH2CHMe)NHCH2Ph given] was saponified with aqueous NaOH in Me2CHOH (82%) and the product was refluxed with SOCl2 in PhMe to give 85% 2,3,4,5-tetrahydro-3-methyl-9-nitro-4-benzyl-1H-1,4-benzodiazepin-5-one. The latter was reduced with LiAlH4 (87.6%) and the product was heated with urea at 210-220° to give 11.5% imidazobenzodiazepinone derivative, which was hydrogenolyzed in HOAc over Pd/C to give 66.8% 4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one. The latter was heated with Na2CO3, KI, and 2,3-dibromopropene in DMF to give title compound III. I had ED50's of 0.032-0.006 µg/mL against HIV-1 in MT-4 cells.

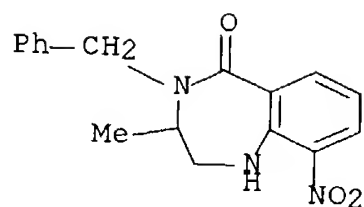
IT **126234-15-9P 126234-17-1P 131645-80-2P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for imidazobenzodiazepinone virucide)

RN 126234-15-9 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

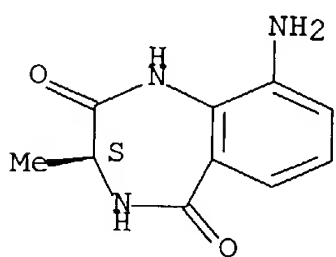


RN 126234-17-1 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)-  
(9CI)

(CA INDEX NAME)

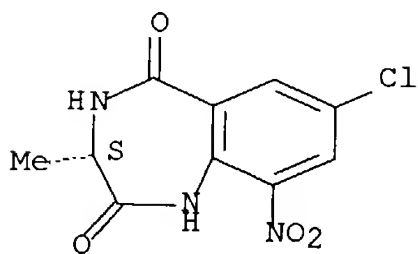
Absolute stereochemistry.



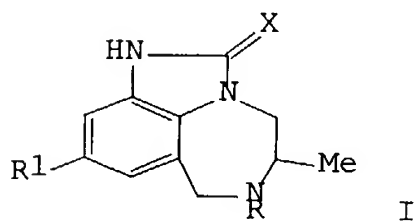
RN 131645-80-2 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 7-chloro-3,4-dihydro-3-methyl-9-nitro-,  
(S)- (9CI) (CA INDEX NAME)

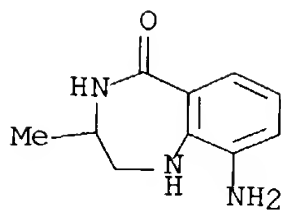
Absolute stereochemistry.



L4 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1991:632195 CAPLUS Full-text  
 DN 115:232195  
 TI Synthesis and anti-HIV-1 activity of 4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) derivatives.  
 2  
 AU Kukla, Michael J.; Breslin, Henry J.; Diamond, Craig J.; Grous, Philip P.;  
 Ho, Chih Y.; Miranda, Milton; Rodgers, James D.; Sherrill, Ronald G.; De Clercq, Erik; et al.  
 CS Janssen Res. Found., Spring House, PA, 19477, USA  
 SO Journal of Medicinal Chemistry (1991), 34(11), 3187-97  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 GI



AB Potential anti-HIV-1 imidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one I (R = R1 = H, X = O) analogs with variations of the five-membered urea ring were prepared. Although many different rings were synthesized to replace the cyclic urea of I, most were found to be inactive in inhibiting the replication of the HIV-1 virus in MT-4 cells. The exceptions were replacement of the urea oxygen with sulfur or selenium to give the corresponding thio- or selenoureas. These were found to be more active than the oxygen counterparts. A small series of analogs were synthesized and tested which allowed direct comparison of urea and thiourea derivs. Without exception, the latter were always more active than the former. The most active compound (S)(+)-I (R = CH2C:CEt2, R1 = Cl, X = S) was found to inhibit the HIV-1 virus with an IC50 of 0.012  $\mu$ M which is comparable to that of AZT.  
 IT **136722-94-6**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclocondensation of, with formamidine acetate)  
 RN 136722-94-6 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-3-methyl- (9CI)  
 (CA INDEX NAME)



IT **131645-80-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT

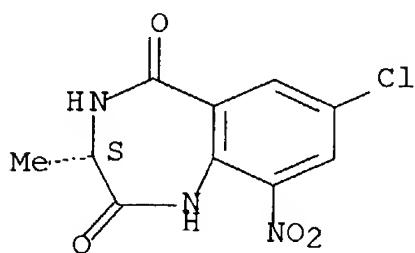
(Reactant or reagent)

(preparation and reduction of)

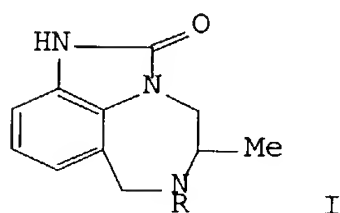
RN 131645-80-2 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 7-chloro-3,4-dihydro-3-methyl-9-nitro-,  
 (S)- (9CI) (CA INDEX NAME)

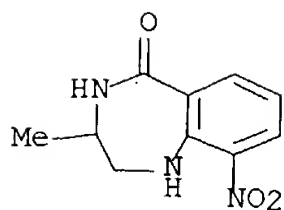
Absolute stereochemistry.



L4 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1991:101957 CAPLUS Full-text  
 DN 114:101957  
 TI Synthesis and anti-HIV-1 activity of 4,5,6,7-tetrahydro-5-methylimidazo[4,5,1-jk][1,4]benzodiazepin-2(1H)-one (TIBO) derivatives  
 AU Kukla, Michael J.; Breslin, Henry J.; Pauwels, Rudi; Fedde, Cynthia L.; Miranda, Milton; Scott, Malcolm K.; Sherrill, Ronald G.; Raeymaekers, Alfons; Van Gelder, Jozef; et al.  
 CS Janssen Res. Found., Spring House, PA, 19477, USA  
 SO Journal of Medicinal Chemistry (1991), 34(2), 746-51  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 OS CASREACT 114:101957  
 GI



AB Title compds. I (R = alkenyl, alkyl, heterocycloalkyl, etc.) have been synthesized and tested for their ability to inhibit the replication of the HIV-1 virus in MT-4 cells. Two synthetic methods are described, one of which allows the synthesis of single enantiomers of the final products. A structure-activity study was done within the series of compds. to determine the optimum group for the 6-position substitution and to determine whether the activity was enantiospecific at the 5-position, which was substituted with a Me group. The best analog, (S)-(+)-I (R = CH<sub>2</sub>CH: CMe<sub>2</sub>), inhibited HIV-1 with an IC<sub>50</sub> (concentrate required to protect 50% of the cells against HIV-1-induced cytopathic effects) of 4 μM, which is comparable to the activity level of DDI, a 2',3'-dideoxynucleoside-type structure undergoing clin. trials as an anti AIDS therapy.  
 IT **131514-78-8P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);  
 RACT (Reactant or reagent)  
       (preparation and reduction of)  
 RN 131514-78-8 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro- (9CI)  
    (CA INDEX NAME)



IT **126234-17-1P**

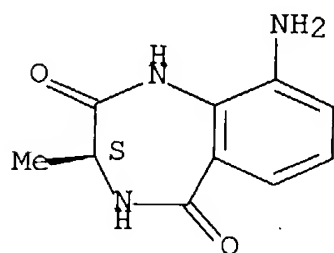
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and sequential reduction and cyclocondensation with  
 trichloromethyl  
 chloroformate)

RN 126234-17-1 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)-  
 (9CI)

(CA INDEX NAME)

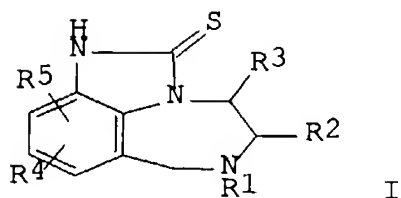
Absolute stereochemistry.



L4 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1991:62128 CAPLUS Full-text  
 DN 114:62128  
 TI Preparation of antiviral tetrahydroimidazo [1,4] benzodiazepin-2-thiones  
 IN Kukla, Michael Joseph; Breslin, Henry Joseph; Raeymaekers, Alfons Herman  
 PA Janssen Pharmaceutica N. V., Belg.  
 SO Eur. Pat. Appl., 30 pp.  
 CODEN: EPXXDW  
 DT Patent  
 LA English  
 FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 384522	A1	19900829	EP 1990-200348	19900216
	EP 384522	B1	19930113		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL				
	IL 93136	A1	19950124	IL 1990-93136	19900123
	AT 84534	E	19930115	AT 1990-200348	19900216
	ES 2046671	T3	19940201	ES 1990-200348	19900216
	CA 2010639	AA	19900823	CA 1990-2010639	19900222
	CA 2010639	C	20010417		
	NO 9000848	A	19900824	NO 1990-848	19900222
	NO 173503	B	19930913		
	NO 173503	C	19931222		
	AU 9050038	A1	19900830	AU 1990-50038	19900222
	AU 617926	B2	19911205		
	JP 02270876	A2	19901105	JP 1990-39883	19900222
	JP 2588624	B2	19970305		
	HU 54158	A2	19910128	HU 1990-896	19900222
	HU 204831	B	19920228		
	DD 293119	A5	19910822	DD 1990-338060	19900222
	ZA 9001366	A	19911030	ZA 1990-1366	19900222
	CS 275171	B2	19920219	CS 1990-854	19900222
	HU 60742	A2	19921028	HU 1991-3076	19900222
	HU 207322	B	19930329		
	PL 163722	B1	19940429	PL 1990-283921	19900222
	FI 92830	B	19940930	FI 1990-897	19900222
	FI 92830	C	19950110		
	RU 2024523	C1	19941215	RU 1990-4743129	19900222
	CN 1045105	A	19900905	CN 1990-100881	19900223
	CN 1029848	B	19950927		
	US 5270464	A	19931214	US 1993-42858	19930405
	US 5371079	A	19941206	US 1993-132030	19931005
	US 6201119	B1	20010313	US 1994-304951	19941017
PRAI	GB 1989-4108	A	19890223		
	GB 1989-20354	A	19890908		
	US 1989-406626	A	19890913		
	GB 1988-6449	A	19880318		
	US 1989-323585	B2	19890314		
	US 1989-406625	B2	19890913		
	US 1990-476926	B2	19900208		
	EP 1990-200348	A	19900216		
	HU 1990-896	A3	19900222		
	US 1990-549349	B2	19900706		
	US 1990-549777	B2	19900709		
	US 1990-583533	B2	19900917		

	US 1991-671238	B1	19910319
	US 1993-42858	A3	19930405
	US 1993-132030	A3	19931005
OS	MARPAT 114:62128		
GI			

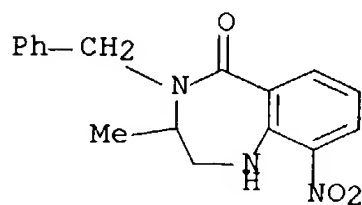


AB The title compds. [I; R1 = alkyl, alkenyl, alkynyl, cycloalkyl, arylalkyl, cycloalkylalkyl; R2, R3 = H, alkyl; R4, R5 = H, alkyl, halo, cyano, NO<sub>2</sub>, CF<sub>3</sub>, OH, alkoxy, amino], were prepared. Thus, a mixture of 6-chloro-2H-3,1-benzoxazine-2,4(1H)dione and alanine Me ester hydrochloride was refluxed 10 h to give 52-58% S-7-chloro-3,4-dihydro-3-methyl-1H-1,4-benzodiazepine-2,5-dione. The latter was treated with HNO<sub>3</sub> at 0° to give the 9-nitro compound, which was converted to S-2,9-dichloro-4,5,6,7-tetrahydro-5-methyl-6-(3-methyl-2-butenyl)imidazo[4,5,6-jk]benzodiazepine, which was refluxed with thiourea in EtOH to give I (R1 = CH<sub>2</sub>CH: CMe<sub>2</sub>, R2 = Me, R3 = R4 = H, R5 = 9-Cl) (II). II had an ED<sub>50</sub> of 0.0005 µg/mL for inhibition of HIV-1 cytopathic effect on MT-4 cells.

IT **126234-15-9P 126234-17-1P 126262-73-5P**  
**131645-75-5P 131645-80-2P 131645-84-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, as virucide intermediate)

RN 126234-15-9 CAPLUS

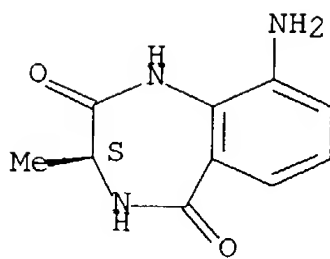
CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 126234-17-1 CAPLUS

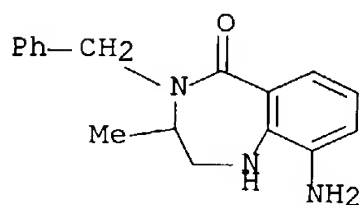
CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)-  
 (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



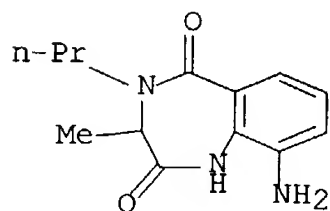
RN 126262-73-5 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-3-methyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 131645-75-5 CAPLUS

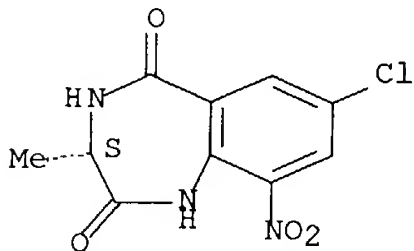
CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-4-propyl- (9CI) (CA INDEX NAME)



RN 131645-80-2 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 7-chloro-3,4-dihydro-3-methyl-9-nitro-, (S)- (9CI) (CA INDEX NAME)

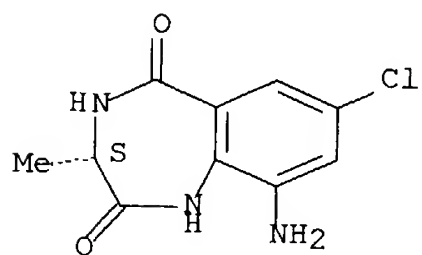
Absolute stereochemistry.



RN 131645-84-6 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-7-chloro-3,4-dihydro-3-methyl-,  
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1990:179038 CAPLUS Full-text

DN 112:179038

TI Preparation and formulation of antiviral  
tetrahydroimidazo[1,4]benzodiazep  
in-2-ones

IN Raeymaekers, Alfons H. M.; Van Gelder, Josephus L. H.; Kukla, Michael  
J.;

Breslin, Henry J.; Janssen, Paul A. J.

PA Janssen Pharmaceutica N. V., Belg.

SO Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

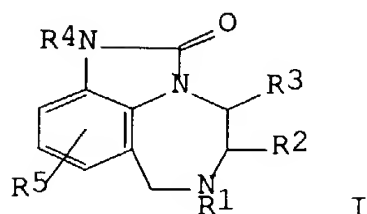
DT Patent

LA English

FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	EP 336466	A1	19891011	EP 1989-200575	19890308
	EP 336466	B1	19921230		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AT 84035	E	19930115	AT 1989-200575	19890308
	ES 2053946	T3	19940801	ES 1989-200575	19890308
	AU 8931310	A1	19890921	AU 1989-31310	19890314
	AU 617435	B2	19911128		
	JP 01275582	A2	19891106	JP 1989-59859	19890314
	HU 52099	A2	19900628	HU 1989-1240	19890316
	HU 203757	B	19910930		
	CA 1310964	A1	19921201	CA 1989-593935	19890316
	DK 8901309	A	19890919	DK 1989-1309	19890317
	FI 8901279	A	19890919	FI 1989-1279	19890317
	FI 89800	B	19930813		
	FI 89800	C	19931125		
	NO 8901176	A	19890919	NO 1989-1176	19890317
	NO 167737	B	19910826		
	NO 167737	C	19911204		
	ZA 8902062	A	19901128	ZA 1989-2062	19890317
	SU 1748647	A3	19920715	SU 1989-4613664	19890317
	CN 1036957	A	19891108	CN 1989-101474	19890318
	CN 1031058	B	19960221		
	KR 133073	B1	19980417	KR 1989-3388	19890318
	NO 9101970	A	19890919	NO 1991-1970	19910522
	NO 179369	B	19960617		
	NO 179369	C	19960925		
	AU 9183602	A1	19911107	AU 1991-83602	19910902
	AU 630575	B2	19921029		
	US 5371079	A	19941206	US 1993-132030	19931005
	US 6201119	B1	20010313	US 1994-304951	19941017
PRAI	GB 1988-6449	A	19880318		
	GB 1989-4108	A	19890223		
	EP 1989-200575	A	19890308		
	US 1989-323585	B2	19890314		
	NO 1989-1176	A1	19890317		
	GB 1989-20354	A	19890908		
	US 1989-406625	B2	19890913		
	US 1989-406626	B2	19890913		
	US 1990-476926	B2	19900208		
	US 1990-549349	B2	19900706		

US 1990-549777	B2	19900709
US 1990-583533	B2	19900917
US 1991-671238	B1	19910319
US 1993-42858	A3	19930405
US 1993-132030	A3	19931005
OS MARPAT 112:179038		
GI		



AB Title compds. I [R1 = H, C1-8 alkyl, C3-6 alkenyl, C3-6 alkynyl, C1-6 alkylcarbonyl, C3-6 cycloalkyl, substituted C1-6 alkyl; R2 = H, C1-6 alkyl, C3-6 alkenyl; R3 = H, C1-6 alkyl; R4 = H, (un)substituted C1-6 alkyl, C1-6 alkoxy carbonyl, C1-6 alkylcarbonyls, C3-6 alkenyl, C3-6 cycloalkyl, C5-6 cycloalkenyl; R5 = H, C1-6 alkyl, halo, (un)substituted Ph] useful as antiviral agents (no data) are prepared 9-Amino-2,3,4,5-tetrahydro-3-methyl-4-(phenylmethyl)-1H-benzodiazepin-5-one (preparation given) and urea were heated to 210-220°, the reaction mixture boiled with HCl, alkalized with NH4OH to give 11.5% I (R1 = PhCH2; R2 = Me; R3-R5 = H).

IT **126234-15-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

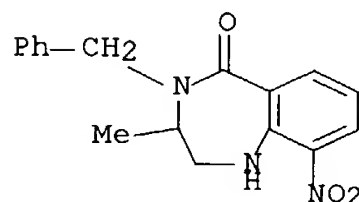
RACT

(Reactant or reagent)

(preparation and reduction of)

RN 126234-15-9 CAPLUS

CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-3-methyl-9-nitro-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT **126234-17-1P 126262-73-5P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for  
tetrahydroimidazobenzodiazepinone  
virucides)

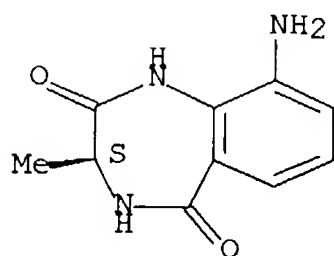
RN 126234-17-1 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 9-amino-3,4-dihydro-3-methyl-, (S)-

(9CI)

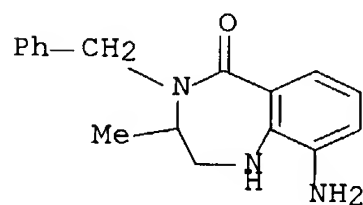
(CA INDEX NAME)

Absolute stereochemistry.

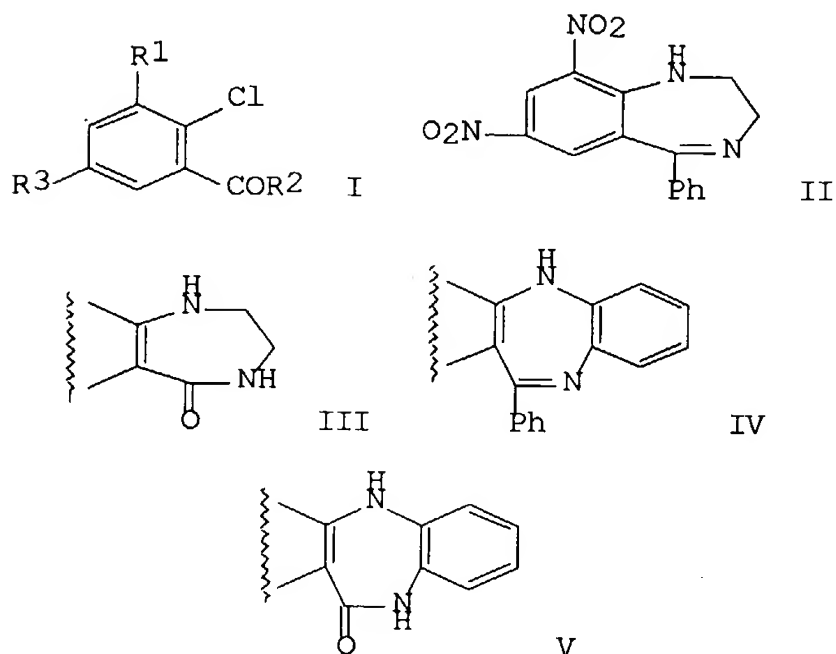


RN 126262-73-5 CAPLUS

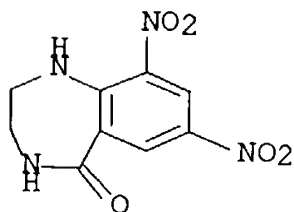
CN 5H-1,4-Benzodiazepin-5-one, 9-amino-1,2,3,4-tetrahydro-3-methyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



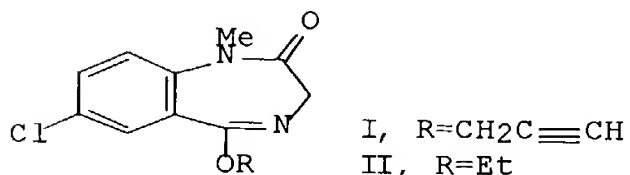
L4 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1988:492960 CAPLUS Full-text  
 DN 109:92960  
 TI Synthesis and structure of 7,9-dinitro-5-phenyl-1,4-benzodiazepine derivatives and benzo[b] analogs  
 AU Dvorkin, A. A.; Simonov, Yu. A.; Ivanov, E. I.; Fedorova, G. V.; Ivanova, R. Yu.  
 CS Fiz. Khim. Inst., Odessa, USSR  
 SO Zhurnal Obshchei Khimii (1987), 57(11), 2613-17  
 CODEN: ZOKHA4; ISSN: 0044-460X  
 DT Journal  
 LA Russian  
 OS CASREACT 109:92960  
 GI



AB Cyclocondensation of o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> and H<sub>2</sub>NCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> with benzoic acid derivs. I (R<sub>1</sub> = R<sub>3</sub> = NO<sub>2</sub>, R<sub>2</sub> = Ph, OMe) gave 65 and 72% benzodiazepines II and III and 68 and 79% benzo[b]-analogs IV and V.  
 IT **115846-71-4P**  
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)  
 RN 115846-71-4 CAPLUS  
 CN 5H-1,4-Benzodiazepin-5-one, 1,2,3,4-tetrahydro-7,9-dinitro- (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1977:415700 CAPLUS Full-text  
 DN 87:15700  
 TI Synthesis and central nervous system evaluation of some  
 5-alkoxy-3H-1,4-benzodiazepin-2(1H)-ones  
 AU Gogerty, John H.; Griot, Rudolf G.; Habeck, Dietmar; Iorio, Louis C.;  
 Houlihan, William J.  
 CS Res. Dev. Div., Sandoz Inc., East Hanover, NJ, USA  
 SO Journal of Medicinal Chemistry (1977), 20(7), 952-6  
 CODEN: JMCMAR; ISSN: 0022-2623  
 DT Journal  
 LA English  
 OS CASREACT 87:15700  
 GI



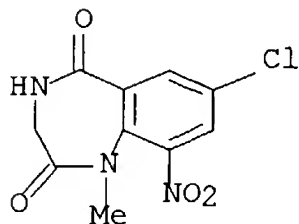
AB A series of 18 title compds. was prepared by treating a 3H-1,4-benzodiazepine-2,5(1H,4H)-dione derivative with a trialkyloxonium fluoroborate, or reacting 5,7-dichloro-1-methyl-3H-1,4-benzodiazepin-2(1H)-one [56967-27-2] with a Na alkoxide or aryloxide. 7-Chloro-1-methyl-5-(propargyloxy)-3H-1,4-benzodiazepin-2(1H)-one (I) [62903-59-7] had the most significant activity in the behavioral studies relative to diazepam. 7-Chloro-5-ethoxy-1-methyl-3H-1,4-benzodiazepin-2(1H)-one (II) [20430-79-9] had the best anticonvulsant activity and had a profile and activity level similar to diazepam in mice. Structure-activity relations are discussed.

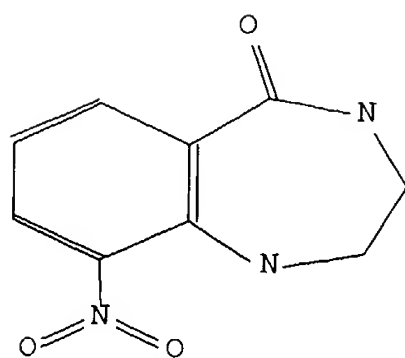
IT **62903-67-7P**

RL: BAC (Biological activity or effector, except adverse); BSU  
 (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (preparation and central nervous system activity of)

RN 62903-67-7 CAPLUS

CN 1H-1,4-Benzodiazepine-2,5-dione, 7-chloro-3,4-dihydro-1-methyl-9-nitro-  
 (9CI) (CA INDEX NAME)

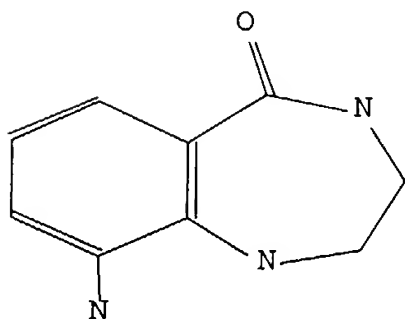




Reference(s):

1. Skalitzky, Donald J.; Marakovits, Joseph T.; Maegley, Karen A.; Ekker, Anne; Yu, Xiao-Hong; Hostomsky, Zdenek; Webber, Stephen E.; Eastman, Brian W.; Almassay, Robert; Li, Jianke; Curtin, Nicola J.; et al., J.Med.Chem., CODEN: JMCMAR, 46(2), <2003>, 210 - 213; BABS-6372884

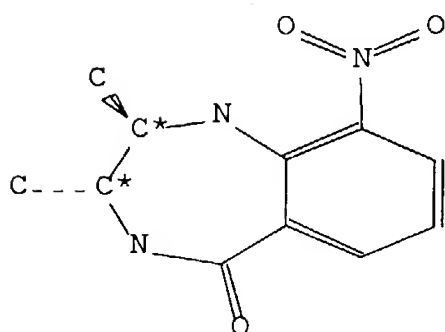
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Autonom Name (AUN):	9-amino-1,2,3,4-tetrahydro- benzo<e><1,4>diazepin-5-one
Molec. Formula (MF):	C9 H11 N3 O
Molecular Weight (MW):	177.21
Lawson Number (LN):	29713
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	7820399
Tautomer ID (TAUTID):	8703386
Entry Date (DED):	2003/04/17
Update Date (DUPD):	2003/04/17



Reference(s):

1. Skalitzy, Donald J.; Marakovits, Joseph T.; Maegley, Karen A.;  
Ekker,  
Anne; Yu, Xiao-Hong; Hostomsky, Zdenek; Webber, Stephen E.; Eastman,  
Brian W.; Almassay, Robert; Li, Jianke; Curtin, Nicola J.; et al.,  
J.Med.Chem., CODEN: JMCMAR, 46(2), <2003>, 210 - 213; BABS-6372884

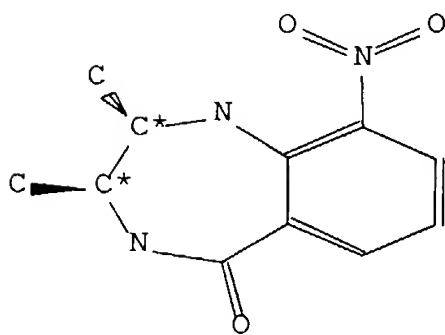
Beilstein Records (BRN):	7337975
Chemical Name (CN):	trans-1,2,3,4-tetrahydro-2,3-dimethyl-9-nitro-5H-1,4-benzodiazepin-5-one
Autonom Name (AUN):	2,3-dimethyl-9-nitro-1,2,3,4-tetrahydro-benzo<e><1,4>diazepin-5-one
Molec. Formula (MF):	C11 H13 N3 O3
Molecular Weight (MW):	235.24
Lawson Number (LN):	28685
File Segment (FS):	racemate, Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6255809
Tautomer ID (TAUTID):	6943649
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1996/02/01
Update Date (DUPD):	1996/11/12



Reference(s):

1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

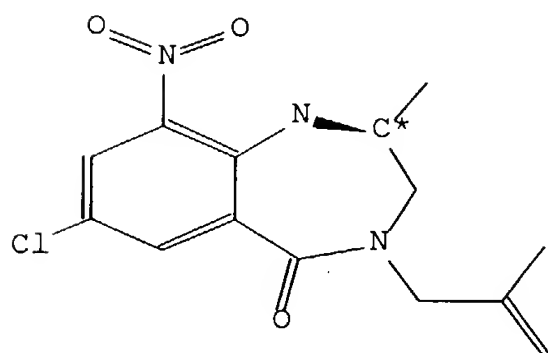
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Chemical Name (CN):	cis-1,2,3,4-tetrahydro-2,3-dimethyl-9-nitro-5H-1,4-benzodiazepin-5-one
Autonom Name (AUN):	2,3-dimethyl-9-nitro-1,2,3,4-tetrahydro-benzo<e><1,4>diazepin-5-one
Molec. Formula (MF):	C11 H13 N3 O3
Molecular Weight (MW):	235.24
Lawson Number (LN):	28685
File Segment (FS):	racemate, Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6255809
Tautomer ID (TAUTID):	6943649
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1996/02/01
Update Date (DUPD):	1996/11/12



Reference(s):

1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

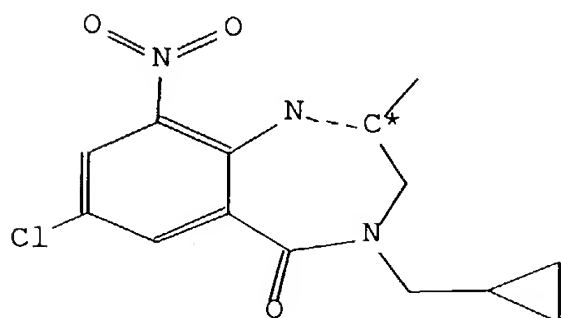
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Chemical Name (CN): (+)-(S)-7-chloro-1,2,3,4-tetrahydro-2-methyl-4-(2-methyl-2-propenyl)-9-nitro-5H-1,4-benzodiazepin-5-one  
Autonom Name (AUN): 7-chloro-2-methyl-4-(2-methyl-allyl)-9-nitro-1,2,3,4-tetrahydro-benzo<e><1,4>diazepin-5-one  
Molec. Formula (MF): C14 H16 Cl N3 O3  
Molecular Weight (MW): 309.75  
Lawson Number (LN): 28676, 2957  
File Segment (FS): Stereo compound  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 6273910  
Tautomer ID (TAUTID): 6967109  
Beilstein Citation (BSO): 6-24  
Entry Date (DED): 1996/02/01  
Update Date (DUPD): 1996/11/12



Reference(s):

1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

Beilstein Records (BRN):	7306711
Chemical Name (CN):	(-)-(R)-7-chloro-4-(cyclopropylmethyl)- 1,2,3,4-tetrahydro-2-methyl-9-nitro-5H- 1,4-benzodiazepin-5-one
Autonom Name (AUN):	7-chloro-4-cyclopropylmethyl-2-methyl-9- nitro-1,2,3,4-tetrahydro- benzo<e><1,4>diazepin-5-one
Molec. Formula (MF):	C14 H16 Cl N3 O3
Molecular Weight (MW):	309.75
Lawson Number (LN):	28676, 14006
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6273902
Tautomer ID (TAUTID):	6967105
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1996/02/01
Update Date (DUPD):	1996/11/12



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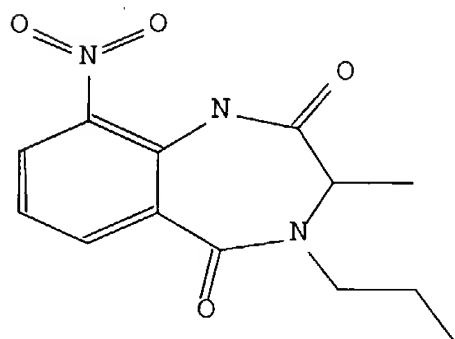
1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

Reference(s) :

1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

L6 ANSWER 7 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7304936
Chemical Name (CN):	3-methyl-9-nitro-4-propyl-3,4-dihydro-
1H-	
Autonom Name (AUN):	benzo<e><1,4>diazepine-2,5-dione
1H-	3-methyl-9-nitro-4-propyl-3,4-dihydro-
Molec. Formula (MF):	benzo<e><1,4>diazepine-2,5-dione
Molecular Weight (MW):	C13 H15 N3 O4
Lawson Number (LN):	277.28
Compound Type (CTYPE):	28852, 2835
Constitution ID (CONSID):	heterocyclic
Tautomer ID (TAUTID):	6264430
Beilstein Citation (BSO):	6963237
Entry Date (DED):	6-24
Update Date (DUPD):	1996/02/01
	1996/11/12

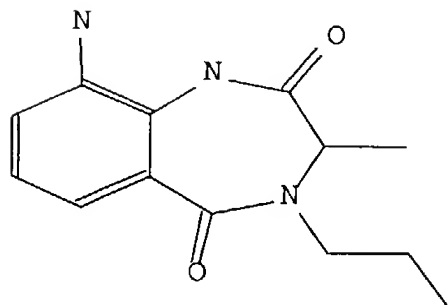


Reference(s):

1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

L6 ANSWER 8 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

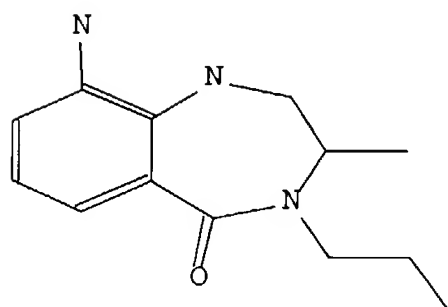
Beilstein Records (BRN):	7298551
Chemical Name (CN):	9-amino-3-methyl-4-propyl-1H-1,4-benzodiazepine-2,5(3H,4H)-dione
Autonom Name (AUN):	9-amino-3-methyl-4-propyl-3,4-dihydro-1H-benzo<e><1,4>diazepine-2,5-dione
Molec. Formula (MF):	C13 H17 N3 O2
Molecular Weight (MW):	247.30
Lawson Number (LN):	29772, 2835
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6197171
Tautomer ID (TAUTID):	6871942
Beilstein Citation (BSO):	6-25
Entry Date (DED):	1996/02/01
Update Date (DUPD):	1996/11/12



Reference(s):  
1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.; Mohrbacher, Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5), <1995>, 771-793; BABS-5970145

L6 ANSWER 9 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

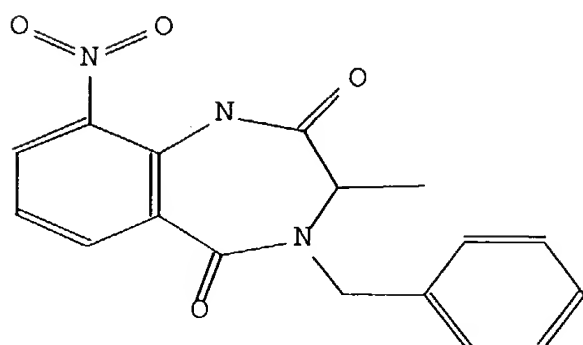
Beilstein Records (BRN): 7293927  
Chemical Name (CN): 9-amino-2,3-dihydro-3-methyl-4-propyl-  
1H-1,4-benzodiazepin-5(4H)-one  
Autonom Name (AUN): 9-amino-3-methyl-4-propyl-1,2,3,4-  
tetrahydro-benzo<e><1,4>diazepin-5-one  
Molec. Formula (MF): C13 H19 N3 O  
Molecular Weight (MW): 233.31  
Lawson Number (LN): 29715, 2835  
Compound Type (CTYPE): heterocyclic  
Constitution ID (CONSID): 6193630  
Tautomer ID (TAUTID): 6866145  
Beilstein Citation (BSO): 6-25  
Entry Date (DED): 1996/02/01  
Update Date (DUPD): 1996/11/12



Reference(s):  
1. Breslin, Henry J.; Kukla, Michael J.; Ludovici, Donald W.;  
Mohrbacher,  
Richard; Ho, Winston; et al., J.Med.Chem., CODEN: JMCMAR, 38(5),  
<1995>, 771-793; BABS-5970145

L6 ANSWER 10 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7225327
Chemical Name (CN):	4-benzyl-3-methyl-9-nitro-1H- <1,4>benzodiazepine-2,5-dione
Autonom Name (AUN):	4-benzyl-3-methyl-9-nitro-3,4-dihydro- 1H-
Molec. Formula (MF):	benzo<e><1,4>diazepine-2,5-dione C17 H15 N3 O4
Molecular Weight (MW):	325.32
Lawson Number (LN):	28852, 14140
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6207667
Tautomer ID (TAUTID):	6879926
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1995/10/31
Update Date (DUPD):	1996/08/09

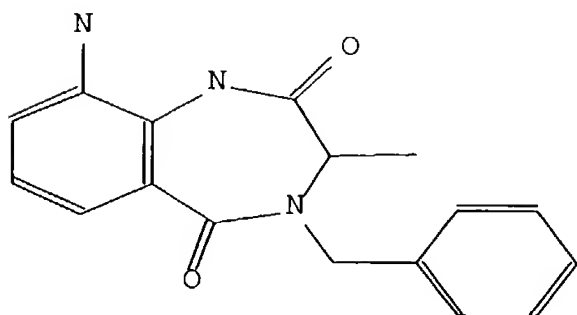


Reference(s):

1. Pfaendler, Hans Rudolf; Weisner, Frank, Heterocycles, CODEN: HTCYAM, 40(2), <1995>, 717-728; BABS-5957554

L6 ANSWER 11 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7218828
Chemical Name (CN):	9-amino-4-benzyl-3-methyl-3,4-dihydro-
1H-	
Autonom Name (AUN):	benzo<e><1,4>diazepine-2,5-dione
1H-	9-amino-4-benzyl-3-methyl-3,4-dihydro-
Molec. Formula (MF):	benzo<e><1,4>diazepine-2,5-dione
Molecular Weight (MW):	C17 H17 N3 O2
Lawson Number (LN):	295.34
Compound Type (CTYPE):	29772, 14140
Constitution ID (CONSID):	heterocyclic
Tautomer ID (TAUTID):	6207498
Beilstein Citation (BSO):	6876551
Entry Date (DED):	6-25
Update Date (DUPD):	1995/10/31
	1996/08/09

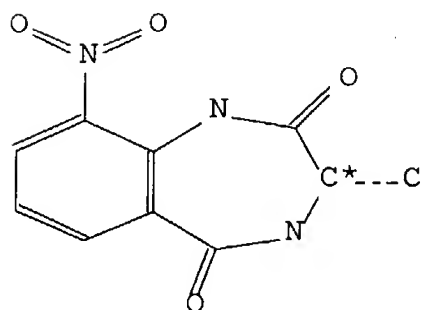


Reference(s):

1. Pfaendler, Hans Rudolf; Weisner, Frank, Heterocycles, CODEN: HTCYAM, 40(2), <1995>, 717-728; BABS-5957554

L6 ANSWER 12 OF 15 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

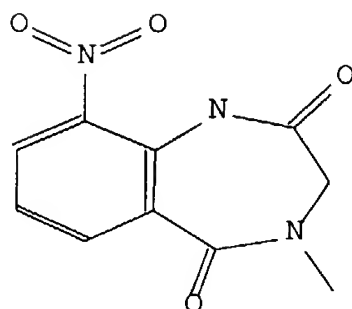
Beilstein Records (BRN):	7215282
Chemical Name (CN):	(+)-(S)-3-methyl-9-nitro-1H- <1,4>benzodiazepine-2,5-dione
Autonom Name (AUN):	3-methyl-9-nitro-3,4-dihydro-1H- benzo<e><1,4>diazepine-2,5-dione
Molec. Formula (MF):	C10 H9 N3 O4
Molecular Weight (MW):	235.20
Lawson Number (LN):	28852
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6194352
Tautomer ID (TAUTID):	6857206
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1995/10/31
Update Date (DUPD):	1996/08/09



Reference(s):

1. Pfaendler, Hans Rudolf; Weisner, Frank, Heterocycles, CODEN: HTCYAM, 40(2), <1995>, 717-728; BABS-5957554

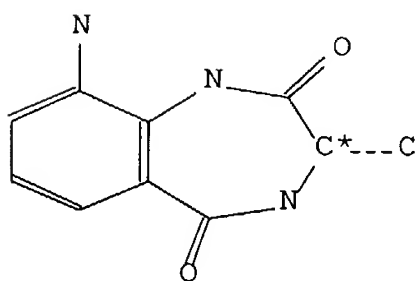
Beilstein Records (BRN):	7215281
Chemical Name (CN):	4-methyl-9-nitro-3,4-dihydro-1H-benzo<e><1,4>diazepine-2,5-dione
Autonom Name (AUN):	4-methyl-9-nitro-3,4-dihydro-1H-benzo<e><1,4>diazepine-2,5-dione
Molec. Formula (MF):	C10 H9 N3 O4
Molecular Weight (MW):	235.20
Lawson Number (LN):	28842, 2817
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6192889
Tautomer ID (TAUTID):	6867986
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1995/10/31
Update Date (DUPD):	1996/08/09



Reference(s):

1. Pfaendler, Hans Rudolf; Weisner, Frank, Heterocycles, CODEN: HTCYAM, 40(2), <1995>, 717-728; BABS-5957554

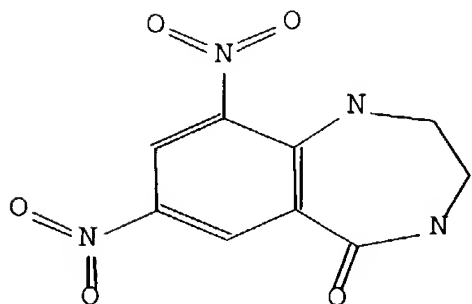
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Chemical Name (CN):	(+)-(S)-9-amino-3-methyl-1H- <1,4>benzodiazepine-2,5-dione
Autonom Name (AUN):	9-amino-3-methyl-3,4-dihydro-1H- benzo<e><1,4>diazepine-2,5-dione
Molec. Formula (MF):	C10 H11 N3 O2
Molecular Weight (MW):	205.22
Lawson Number (LN):	29772
File Segment (FS):	Stereo compound
Compound Type (CTYPE):	heterocyclic
Beilstein Citation (BSO):	6-25
Entry Date (DED):	1995/10/31
Update Date (DUPD):	1996/08/09
Compound Disposition (CDISP):	4295513 Alternate BRN



Reference(s):

1. Pfaendler, Hans Rudolf; Weisner, Frank, Heterocycles, CODEN: HTCYAM, 40(2), <1995>, 717-728; BABS-5957554

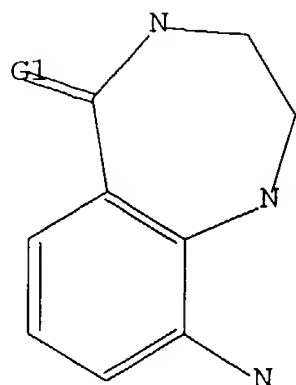
Beilstein Records (BRN):	7098769
Chemical Name (CN):	7,9-dinitro-1,2,4,5-tetrahydro-1H-1,4-benzodiazepin-5-one
Autonom Name (AUN):	7,9-dinitro-1,2,3,4-tetrahydro-benzo<e><1,4>diazepin-5-one
Molec. Formula (MF):	C9 H8 N4 O5
Molecular Weight (MW):	252.19
Lawson Number (LN):	28666
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	6053236
Tautomer ID (TAUTID):	6674329
Beilstein Citation (BSO):	6-24
Entry Date (DED):	1995/05/11
Update Date (DUPD):	1995/05/11



Reference(s):

1. Dvorkin, A. A.; Simonov, Yu. A.; Ivanov, E. I.; Fedorova, G. V.; Ivanova, R.  
Yu., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 57(11), <1987>, 2328-2332, Zh.Obshch.Khim., CODEN: ZOKHA4, 57(11), <1987>, 2613-2617; BABS-5938720

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FILE 'BEILSTEIN' ENTERED AT 17:32:01 ON 25 AUG 2004

L5 23 S L1 FUL  
L6 15 S L5 NOT L4

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